

Palladium-Catalyzed Direct Alkenylation of 2-Methyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-ones Using Oxygen as the Oxidant

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Supporting Information

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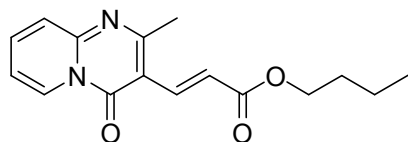
A. General method

All reactions were performed for synthesis of products **3a-3u** at 80 °C in a round bottom flask equipped with oxygen bag and magnetic stir bar. NMR spectra were recorded using a Bruker Avance 400 MHz NMR spectrometer (100 M Hz for carbon) and respectively referenced to 7.26 and 77.0 ppm for chloroform-d solvent with TMS as internal standard. ESI-MS spectra were measured on Finnigan Mat TSQ 7000 instruments. Elemental analyses were performed on a Heraeus elemental analyzer. Melting points were measured with a Tektronix X4 apparatus and are uncorrected. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF₂₅₄), and visualization was effected at 254 nm.

B. General procedure

Synthesis of 3a: 2-methyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one **1a** (80 mg, 0.5 mmol), *n*-butyl acrylate **2a** (128 mg, 1 mmol), Pd(OAc)₂ (11.2 mg, 10 mol%) and PivOH (255 mg, 2.5 mmol) were stirred in 1 mL of DMF equipped with oxygen bag at 80 °C for 24 h. After completion of the reaction (monitored by TLC), the water (10 mL) was added. The aqueous solution was extracted with ethyl acetate (3×10 mL) and the combined extract was dried with anhydrous MgSO₄. The solvent was removed and the crude product was separated by column chromatography (eluted with petroleum ether/ethyl acetate = 2:1) to give a pure sample of **3a** (105 mg, 74% yield).

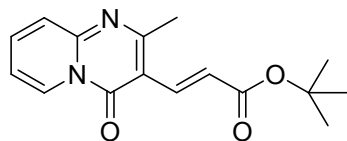
C. Analytical data for 3a-3u



(*E*)-butyl 3-(2-methyl-4-oxo-4*H*-pyrido[1,2-*a*]pyrimidin-3-yl)acrylate(**3a**)

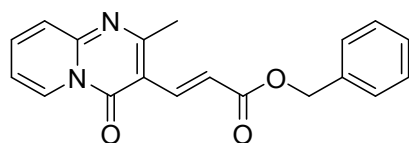
Yellow crystal, m.p. 200-202 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.13 (d, *J* = 6.8 Hz, 1H), 7.85 (d, *J* = 15.6 Hz, 1H), 7.79 (d, *J* = 7.2 Hz, 1H), 7.65 (m, 1H), 7.39 (d, *J* = 15.6 Hz, 1H), 7.22 (t, *J* = 6.8 Hz, 1H), 4.22 (t, *J* = 6.6 Hz, 2H), 2.69 (s, 3H), 1.73-1.66 (m, 2H), 1.50-1.41 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.5, 165.4, 155.7, 149.4, 137.1, 136.5, 127.8, 126.0, 121.1, 116.1, 109.2, 64.2, 30.8,

23.5, 19.2, 13.8. ESI-MS (m/z) 287 [M+H]⁺. Anal. calcd. C, 67.12; H, 6.34; N, 9.78; Found: C, 67.00; H, 6.28; N, 9.65.



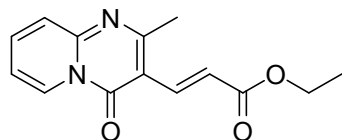
(E)-tert-butyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3b)

Yellow crystal, m.p. 204-205 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.11 (d, *J* = 7.2 Hz, 1H), 7.80-7.75 (m, *J* = 15.6 Hz, *J* = 7.2 Hz, 2H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 15.6 Hz, 1H), 7.20 (t, *J* = 6.8 Hz, 1H), 2.68 (s, 3H), 1.53 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 167.8, 165.0, 155.7, 149.2, 137.0, 135.4, 127.8, 125.9, 123.2, 116.1, 109.1, 80.1, 28.2, 23.3. ESI-MS (m/z) 287 [M+H]⁺. Anal. calcd. C, 67.12; H, 6.34; N, 9.78; Found: C, 67.02; H, 6.29; N, 9.63.



(E)-benzyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3c)

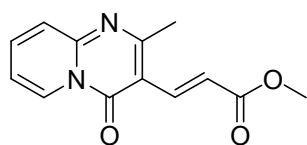
Yellow crystal, m.p. 176-178 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.10 (d, *J* = 6.8 Hz, 1H), 7.89 (d, *J* = 15.6 Hz, 1H), 7.77 (m, 1H), 7.62 (m, 1H), 7.47-7.32 (m, 6H), 7.19 (t, *J* = 7.0 Hz, 1H), 5.27 (s, 2H), 2.68 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.3, 165.6, 155.7, 149.4, 137.2, 136.4, 128.5, 128.1, 128.0, 127.9, 126.1, 120.5, 116.1, 108.8, 66.1, 23.5. ESI-MS (m/z) 321 [M+H]⁺. Anal. calcd. C, 71.24; H, 5.03; N, 8.74; Found: C, 71.10; H, 4.98; N, 8.62.



(E)-ethyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3d)

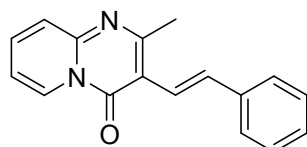
Yellow crystal, m.p. 220-222 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.07 (d, *J* = 6.8 Hz, 1H), 7.82-7.74 (m, *J* = 15.6 Hz, *J* = 6.8 Hz, 2H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.33 (d, *J* = 15.6 Hz, 1H), 7.18 (t, *J* = 6.8 Hz, 1H), 4.23 (q, *J* = 7.2 Hz, 2H), 2.65 (s, 3H), 1.30 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.4, 165.4, 155.7, 149.4, 137.1, 136.5, 127.8, 126.0, 121.0, 116.1, 108.8, 60.3, 23.4, 14.4. ESI-MS (m/z) 259 [M+H]⁺.

Anal. calcd. C, 65.11; H, 5.46; N, 10.85; Found: C, 65.01; H, 5.41; N, 10.73.



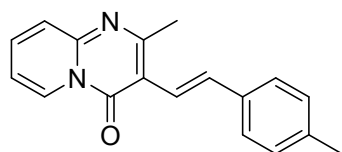
(E)-methyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3e)

Yellow crystal, m.p. 205-206 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.13 (d, *J* = 7.2 Hz, 1H), 7.88-7.78 (m, *J* = 15.6 Hz, *J* = 6.8 Hz, 2H), 7.65 (d, *J* = 9.2 Hz, 1H), 7.40 (d, *J* = 15.6 Hz, 1H), 7.22 (d, *J* = 6.8 Hz, 1H), 3.81 (s, 3H), 2.70 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.8, 165.4, 155.7, 149.4, 137.2, 136.8, 127.9, 126.0, 120.6, 116.1, 108.8, 51.6, 23.4. ESI-MS (*m/z*) 245 [M+H]⁺. Anal. calcd. C, 63.93; H, 4.95; N, 11.47; Found: C, 63.82; H, 4.91; N, 11.35.



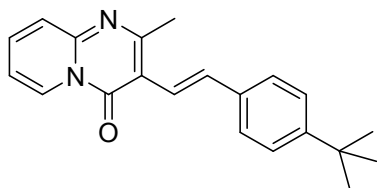
(E)-2-methyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3f)

Yellow crystal, m.p. 213-215 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.14 (d, *J* = 7.2 Hz, 1H), 8.11 (d, *J* = 16.0 Hz, 1H), 7.71-7.67 (m, 1H), 7.63-7.58 (m, 3H), 7.41-7.37 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 16.0 Hz, 1H), 7.17-7.13 (m, 1H), 2.73 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.7, 155.9, 148.0, 138.6, 135.2, 133.3, 128.6, 127.5, 127.2, 126.5, 125.8, 121.1, 115.4, 111.6, 23.5. ESI-MS (*m/z*) 263 [M+H]⁺. Anal. calcd. C, 77.84; H, 5.38; N, 10.68; Found: C, 77.73; H, 5.32; N, 10.75.



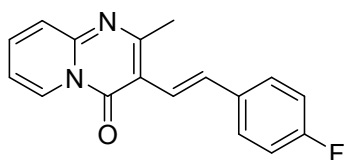
(E)-3-(4-methylstyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3g)

Yellow crystal, m.p. 198-200 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.08 (d, *J* = 7.2 Hz, 1H), 8.04 (d, *J* = 16.4 Hz, 1H), 7.65-7.61 (m, 1H), 7.56 (m, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.16-7.07 (m, 4H), 2.68 (s, 3H), 2.35 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.5, 156.0, 147.9, 137.4, 135.8, 135.1, 133.3, 129.4, 127.2, 126.5, 125.8, 120.2, 115.4, 111.8, 23.6, 21.3. ESI-MS (*m/z*) 277 [M+H]⁺. Anal. calcd. C, 78.24; H, 5.84; N, 10.14; Found: C, 78.11; H, 5.77; N, 10.12.



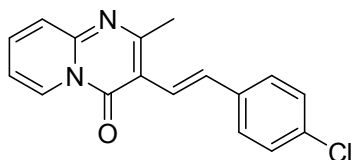
(E)-3-(4-tert-butylstyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3h)

Yellow crystal, m.p. 144-146 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.11 (d, *J* = 7.2 Hz, 1H), 8.06 (d, *J* = 16.0 Hz, 1H), 7.68-7.64 (m, 1H), 7.60 (m, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 16.0 Hz, 1H), 7.14-7.10 (m, 1H), 2.69 (s, 3H), 1.34 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 161.6, 156.0, 150.7, 147.9, 135.8, 135.1, 133.3, 127.2, 126.3, 125.8, 125.6, 120.5, 115.4, 111.9, 34.6, 31.3, 23.5. ESI-MS (*m/z*) 319 [M+H]⁺. Anal. calcd. C, 79.21; H, 6.96; N, 8.80; Found: C, 79.11; H, 6.91; N, 8.68.



(E)-3-(4-fluorostyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3i)

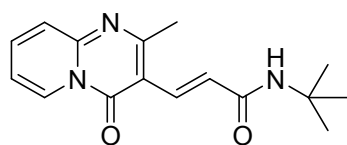
Yellow crystal, m.p. 206-208 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.12 (d, *J* = 7.2 Hz, 1H), 8.05 (d, *J* = 16.0 Hz, 1H), 7.72-7.68 (m, 1H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.54-7.51 (m, 2H), 7.17-7.14 (m, 1H), 7.10 (d, *J* = 16.0 Hz, 1H), 7.07-7.03 (m, 2H), 2.70 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.6, 161.7, 156.0, 148.1, 135.4, 134.8, 132.2, 128.1, 128.0, 127.3, 125.8, 120.9, 115.7, 115.6, 115.5, 111.6, 23.4. ESI-MS (*m/z*) 281 [M+H]⁺. Anal. calcd. C, 72.85; H, 4.67; N, 9.99; Found: C, 72.75; H, 4.61; N, 9.87.



(E)-3-(4-chlorostyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3j)

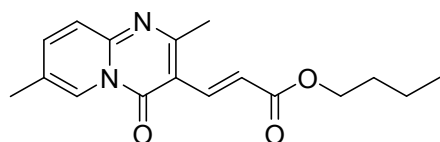
Yellow crystal, m.p. 130-132 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.11 (d, *J* = 7.2 Hz, 1H), 8.05 (d, *J* = 16.4 Hz, 1H), 7.72-7.69 (m, 1H), 7.62 (m, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.18-7.14 (m, 2H), 2.70 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.9, 156.0, 148.1, 137.1, 135.6, 133.1, 131.9, 128.8, 127.7, 127.3, 125.8, 121.7, 115.7, 111.4, 23.5. ESI-MS (*m/z*) 297 [M+H]⁺. Anal. calcd. C, 68.81; H, 4.42;

N, 9.44; Found: C, 68.70; H, 4.37; N, 9.35.



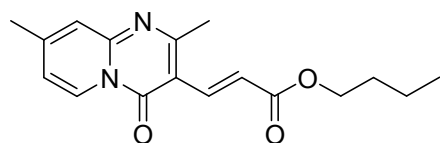
(E)-N-tert-butyl-3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylamide(3k)

Yellow crystal, m.p. 136-138 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.09 (d, *J* = 7.2 Hz, 1H), 7.78-7.74 (m, 2H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.40 (d, *J* = 15.2 Hz, 1H), 7.19 (t, *J* = 6.8 Hz, 1H), 5.65 (s, 1H), 2.70 (s, 3H), 1.44 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 166.4, 165.3, 155.9, 149.0, 136.5, 132.2, 127.5, 126.1, 124.9, 116.0, 109.2, 51.4, 28.9, 23.4. ESI-MS (*m/z*) 286 [M+H]⁺. Anal. calcd. C, 67.35; H, 6.71; N, 14.73; Found: C, 67.25; H, 6.67; N, 14.82.



(E)-butyl 3-(2,7-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3l)

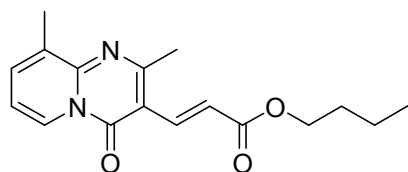
Yellow crystal, m.p. 230-232 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.91 (s, 1H), 7.85 (d, *J* = 15.6 Hz, 1H), 7.65 (dd, *J* = 1.6 Hz, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.37 (d, *J* = 15.6 Hz, 1H), 4.22 (t, *J* = 6.6 Hz, 2H), 2.67 (s, 3H), 2.46 (s, 3H), 1.73-1.66 (m, 2H), 1.50-1.41 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.6, 164.8, 155.6, 148.3, 140.0, 134.0, 136.7, 126.5, 125.5, 125.3, 120.7, 108.5, 64.2, 30.9, 23.4, 19.2, 18.4, 13.8. ESI-MS (*m/z*) 301 [M+H]⁺. Anal. calcd. C, 67.98; H, 6.71; N, 9.33; Found: C, 67.86; H, 6.65; N, 9.20.



(E)-butyl 3-(2,8-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3m)

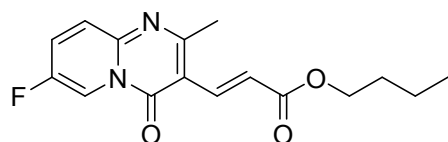
Yellow crystal, m.p. 173-175 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.00 (d, *J* = 7.2 Hz, 1H), 7.83 (d, *J* = 15.2 Hz, 1H), 7.40 (s, 1H), 7.35 (d, *J* = 15.6 Hz, 1H), 7.04 (dd, *J* = 1.6 Hz, *J* = 7.2 Hz, 1H), 4.21 (t, *J* = 6.8 Hz, 2H), 2.66 (s, 3H), 2.51 (s, 3H), 1.73-1.66

(m, 2H), 1.49-1.40 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 168.6, 165.7, 155.7, 149.7, 149.3, 136.7, 127.1, 124.2, 120.3, 118.7, 108.0, 64.1, 30.9, 23.5, 21.5, 19.2, 13.8. ESI-MS (m/z) 301 $[\text{M}+\text{H}]^+$. Anal. calcd. C, 67.98; H, 6.71; N, 9.33; Found: C, 67.87; H, 6.67; N, 9.22.



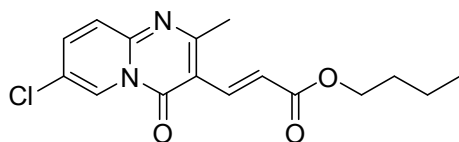
(E)-butyl 3-(2,9-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3n)

Yellow crystal, m.p. 196-198 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.01 (d, $J = 7.2$ Hz, 1H), 7.87 (d, $J = 15.6$ Hz, 1H), 7.62 (d, $J = 6.8$ Hz, 1H), 7.39 (d, $J = 15.2$ Hz, 1H), 7.09 (t, $J = 7.0$ Hz, 1H), 4.21 (t, $J = 6.8$ Hz, 2H), 2.70 (s, 3H), 2.60 (s, 3H), 1.73-1.66 (m, 2H), 1.50-1.40 (m, 2H), 0.96 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 168.7, 164.6, 156.3, 148.8, 136.9, 135.8, 134.9, 125.8, 120.7, 115.5, 108.5, 64.2, 30.9, 23.7, 19.2, 17.9, 13.8. ESI-MS (m/z) 301 $[\text{M}+\text{H}]^+$. Anal. calcd. C, 67.98; H, 6.71; N, 9.33; Found: C, 67.90; H, 6.65; N, 9.21.



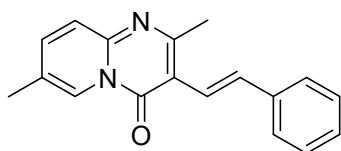
(E)-butyl 3-(7-fluoro-2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3o)

Yellow crystal, m.p. 142-143 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.99 (dd, $J = 2.6$ Hz, 1H), 7.81 (d, $J = 15.6$ Hz, 1H), 7.69-7.64 (m, 2H), 7.37 (d, $J = 15.6$ Hz, 1H), 4.20 (t, $J = 6.6$ Hz, 2H), 2.67 (s, 3H), 1.71-1.64 (m, 2H), 1.48-1.39 (m, 2H), 0.95 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 168.3, 164.8, 155.6, 155.2, 153.2, 147.2, 136.1, 129.3, 129.1, 128.0, 127.9, 121.9, 114.2, 113.8, 108.8, 64.3, 30.8, 23.3, 19.2, 13.7. ESI-MS (m/z) 305 $[\text{M}+\text{H}]^+$. Anal. calcd. C, 63.15; H, 5.63; N, 9.21; Found: C, 63.12; H, 5.57; N, 9.07.



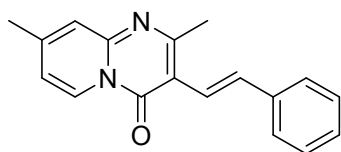
(E)-butyl 3-(7-chloro-2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3p)

Yellow crystal, m.p. 185-187 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.10 (d, *J* = 2.0 Hz, 1H), 7.80 (d, *J* = 15.6 Hz, 1H), 7.70 (dd, *J* = 2.4 Hz, *J* = 9.2 Hz, 1H), 7.56 (d, *J* = 9.2 Hz, 1H), 7.36 (d, *J* = 15.2 Hz, 1H), 4.21 (t, *J* = 6.6 Hz, 2H), 2.66 (s, 3H), 1.72-1.65 (m, 2H), 1.49-1.39 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 168.3, 165.2, 154.8, 147.6, 138.0, 136.0, 127.0, 125.5, 124.7, 121.9, 109.4, 64.3, 30.8, 23.4, 19.2, 13.7. ESI-MS (*m/z*) 321 [M+H]⁺. Anal. calcd. C, 59.91; H, 5.34; N, 8.73; Found: C, 59.80; H, 5.28; N, 8.60.



(E)-2,7-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3q)

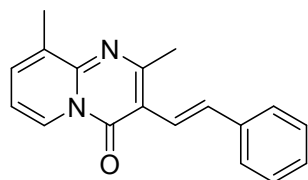
Yellow crystal, m.p. 209-211 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.92 (s, 1H), 8.08 (d, *J* = 16.0 Hz, 1H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 1.2 Hz, 2H), 7.39-7.35 (m, 2H), 7.28-7.24 (m, 1H), 7.20 (d, *J* = 16.0 Hz, 1H), 2.69 (s, 3H), 2.43 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.3, 155.8, 147.0, 138.7, 138.3, 133.0, 128.6, 127.4, 126.5, 125.7, 125.3, 124.7, 121.4, 111.3, 23.5, 18.4. ESI-MS (*m/z*) 277 [M+H]⁺. Anal. calcd. C, 78.24; H, 5.84; N, 10.14; Found: C, 78.14; H, 5.79; N, 10.06.



(E)-2,8-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3r)

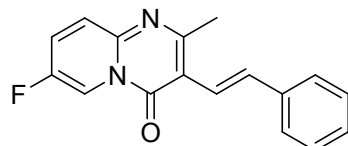
Yellow crystal, m.p. 147-149 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.99 (d, *J* = 7.2 Hz, 1H), 8.02 (d, *J* = 16.0 Hz, 1H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.37-7.33 (m, 3H), 7.26-7.22 (m, 1H), 7.16 (d, *J* = 16.0 Hz, 1H), 6.96-6.94 (m, 1H), 2.67 (s, 3H), 2.44 (s, 3H). ¹³C

NMR (100 MHz, CDCl₃) δ 162.0, 156.0, 148.0, 147.6, 138.7, 132.6, 128.6, 127.4, 126.5, 126.4, 123.8, 121.3, 118.2, 110.7, 23.5, 21.4. ESI-MS (m/z) 277 [M+H]⁺. Anal. calcd. C, 78.24; H, 5.84; N, 10.14; Found: C, 78.12; H, 5.78; N, 10.02.



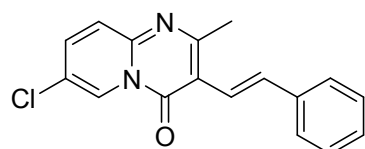
(E)-2,9-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3s)

Yellow crystal, m.p. 197-199 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.00 (d, J = 7.2 Hz, 1H), 8.08 (d, J = 16.0 Hz, 1H), 7.56 (d, J = 7.2 Hz, 2H), 7.48 (d, J = 6.8 Hz, 1H), 7.38-7.34 (m, 2H), 7.25-7.18 (m, 2H), 7.00 (t, J = 7.0 Hz, 1H), 2.71 (s, 3H), 2.58 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.1, 156.5, 147.5, 138.8, 134.5, 134.0, 132.8, 128.6, 127.4, 126.5, 125.3, 121.5, 114.9, 111.1, 23.9, 17.9. ESI-MS (m/z) 277 [M+H]⁺. Anal. calcd. C, 78.24; H, 5.84; N, 10.14; Found: C, 78.13; H, 5.78; N, 10.01.



(E)-7-fluoro-2-methyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3t)

Yellow crystal, m.p. 200-202 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.02-9.00 (m, 1H), 8.10 (d, J = 15.6 Hz, 1H), 7.60-7.56 (m, 4H), 7.40-7.36 (m, 2H), 7.30-7.28 (m, 1H), 7.18 (d, J = 16.0 Hz, 1H), 2.70 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.3, 155.4, 155.4, 152.9, 145.8, 138.3, 134.0, 128.6, 127.8, 127.7, 127.4, 126.6, 120.8, 113.4, 113.0, 111.5, 23.4. ESI-MS (m/z) 281 [M+H]⁺. Anal. calcd. C, 72.85; H, 4.67; F, 6.78; N, 9.99; Found: C, 72.74; H, 4.62; N, 9.86.

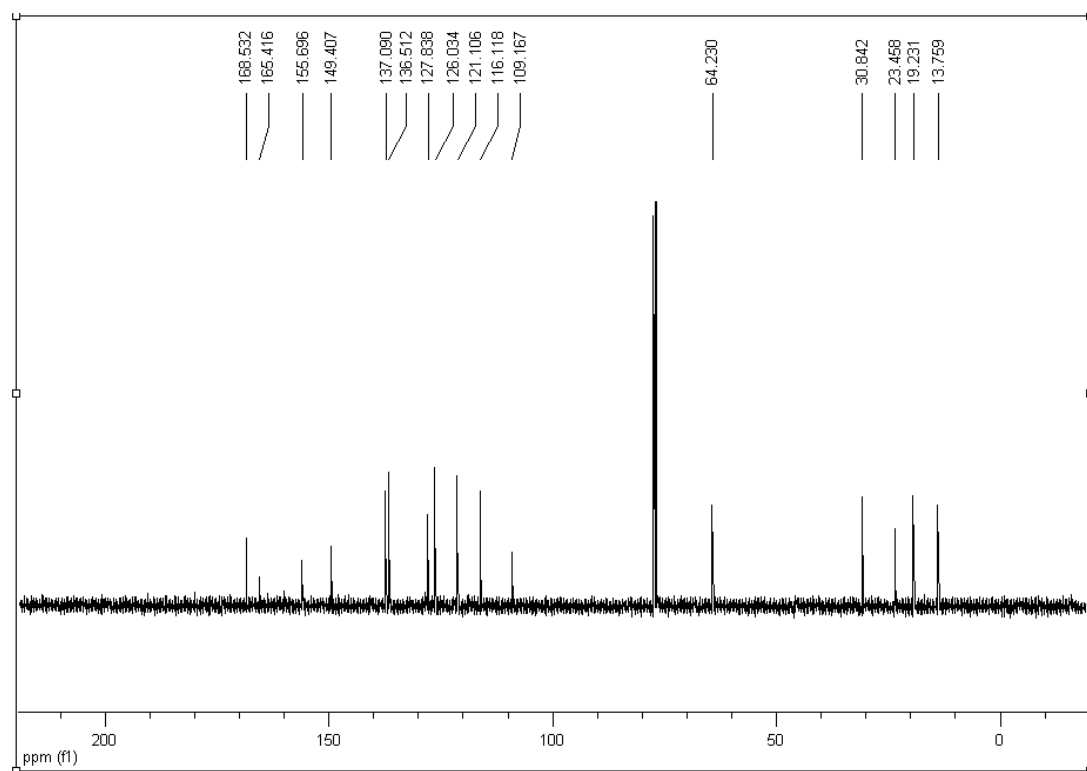
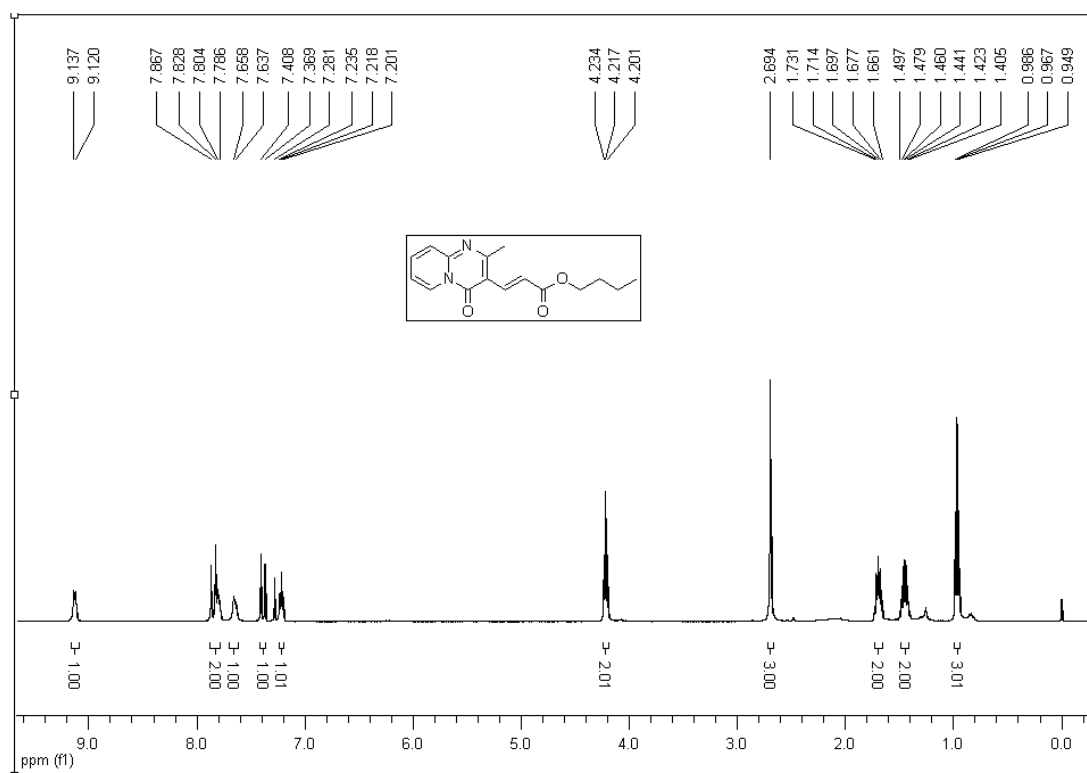


(E)-7-chloro-2-methyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3u)

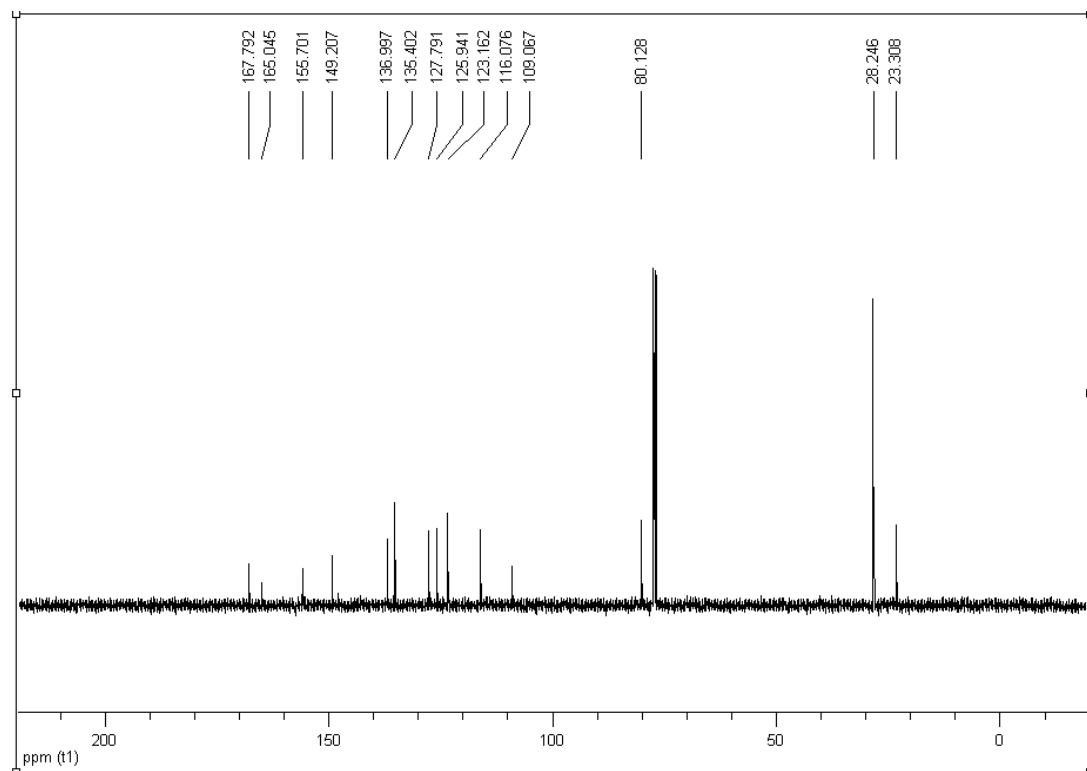
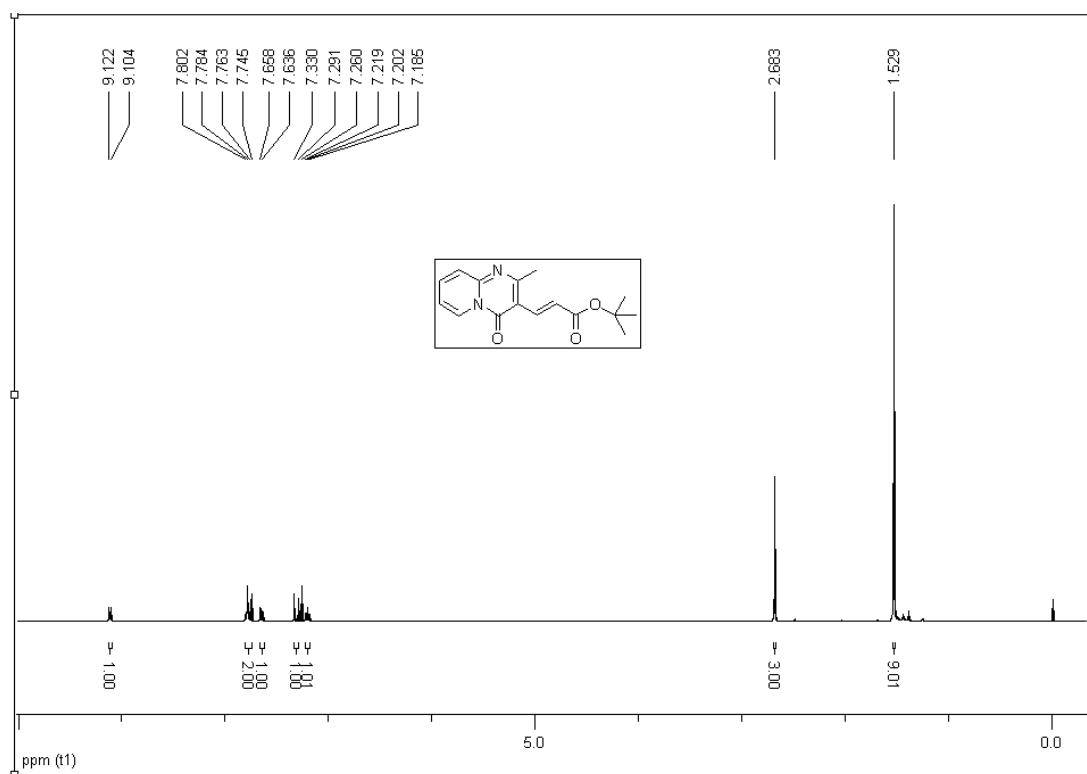
Yellow crystal, m.p. 239-241 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.09 (d, *J* = 2.0 Hz, 1H), 8.05 (d, *J* = 16.0 Hz, 1H), 7.55-7.51 (m, 4H), 7.36-7.32 (m, 2H), 7.24-7.22 (m, 1H), 7.14 (d, *J* = 16.0 Hz, 1H), 2.66 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.5, 155.1, 146.2, 138.3, 136.3, 134.1, 128.6, 127.7, 126.9, 126.6, 125.0, 124.1, 120.7, 112.3, 23.5. ESI-MS (*m/z*) 297 [M+H]⁺. Anal. calcd. C, 68.81; H, 4.42; N, 9.44; Found: C, 68.71; H, 4.17; N, 9.32.

D. NMR spectra

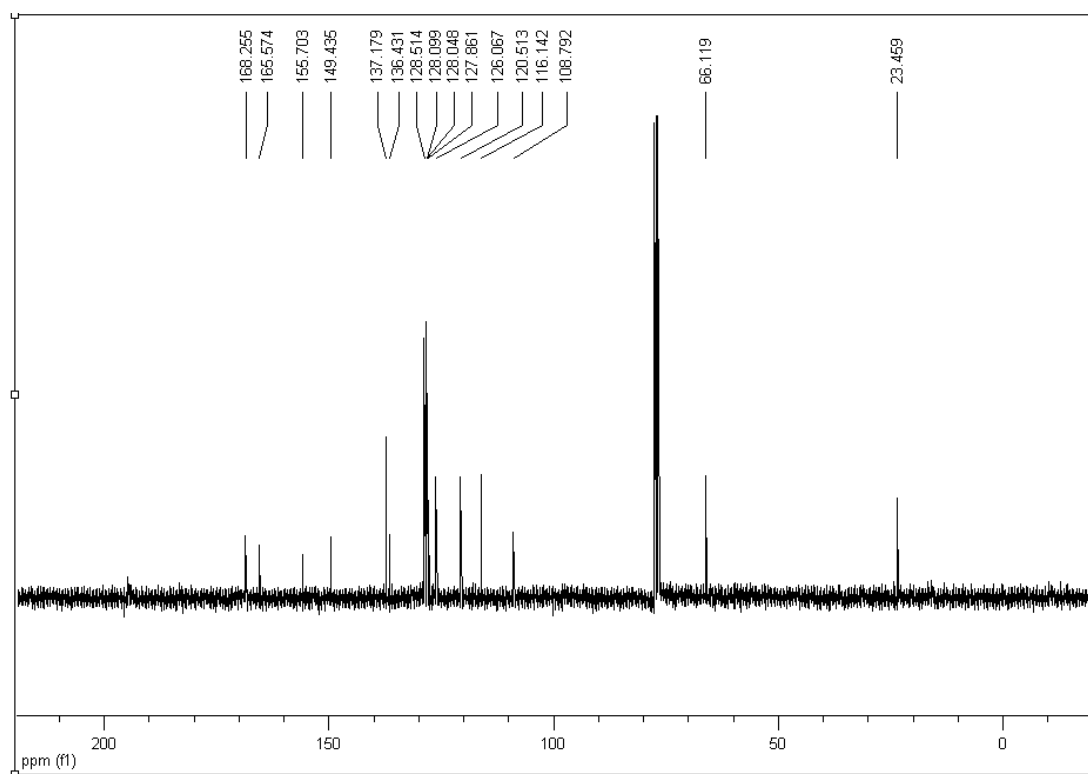
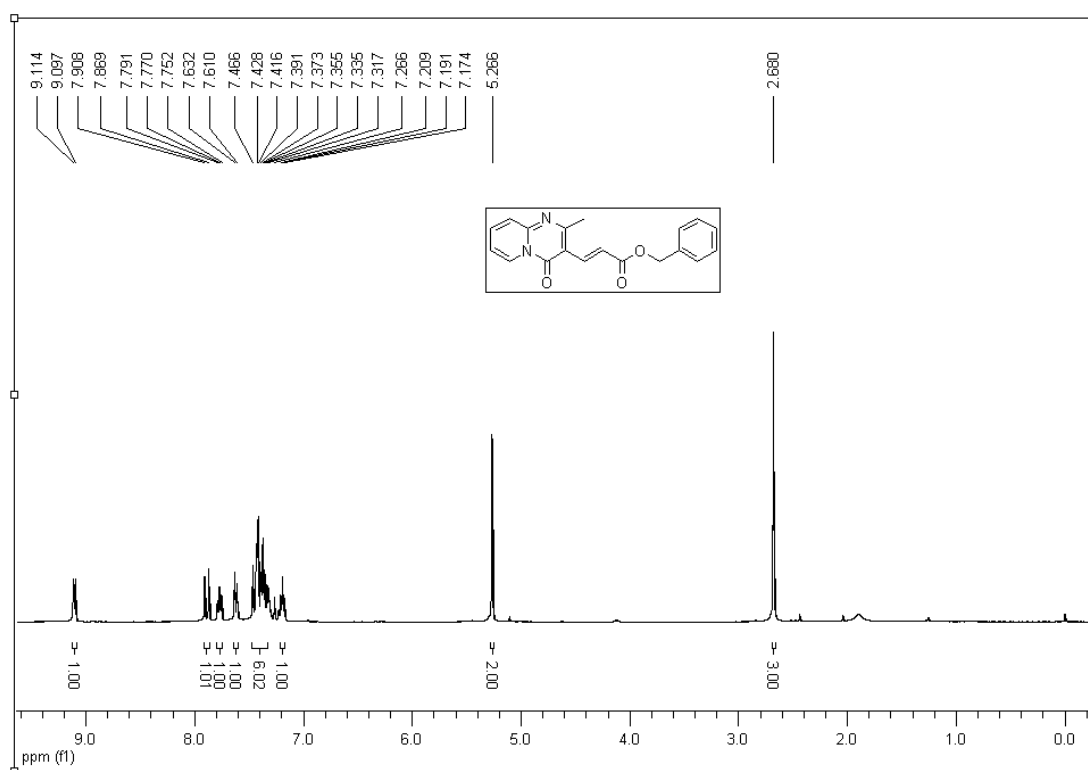
(*E*)-butyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3a)



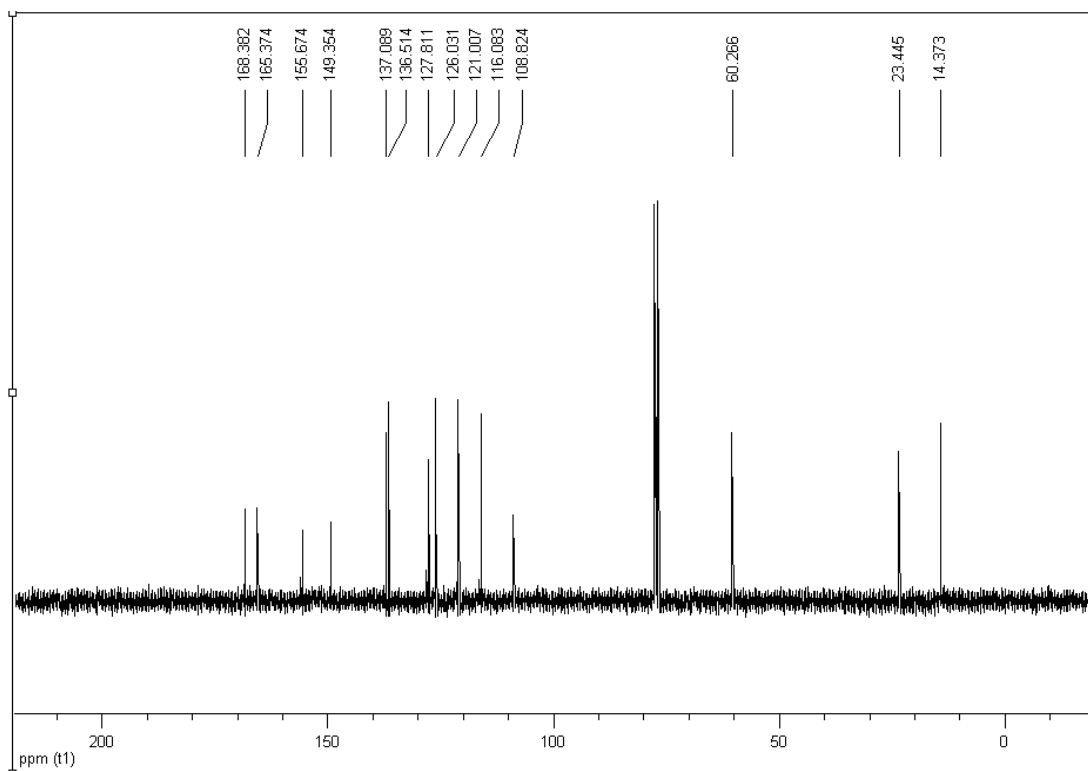
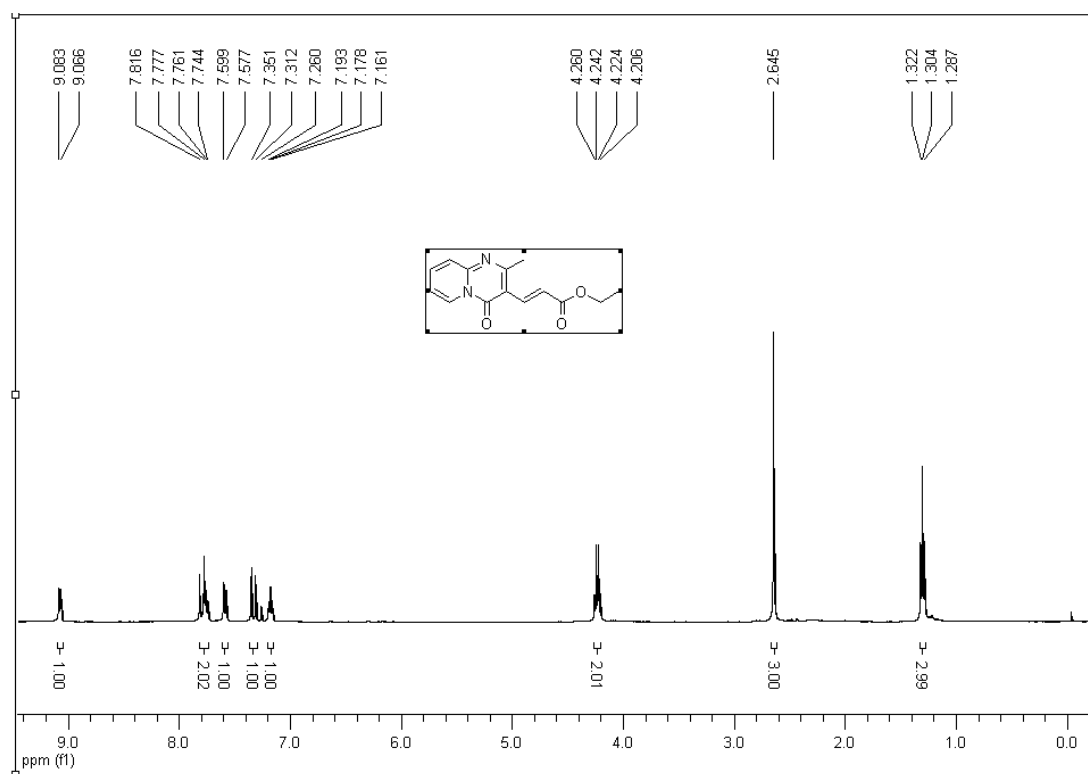
(E)-tert-butyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3b)



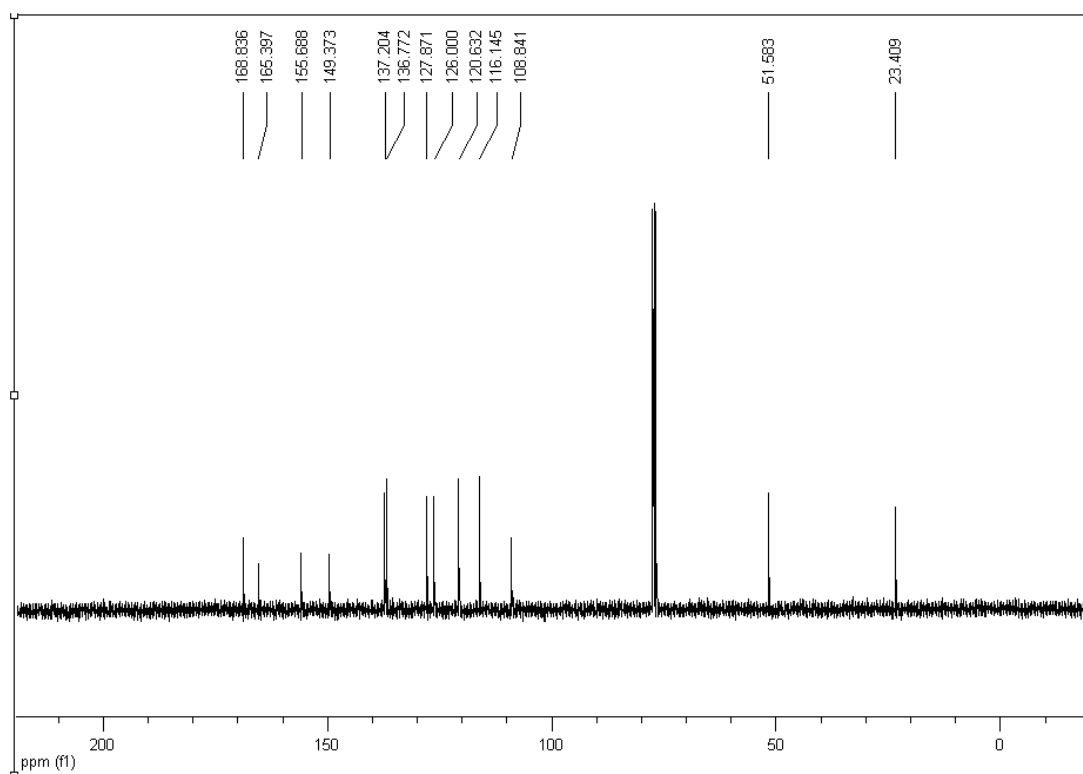
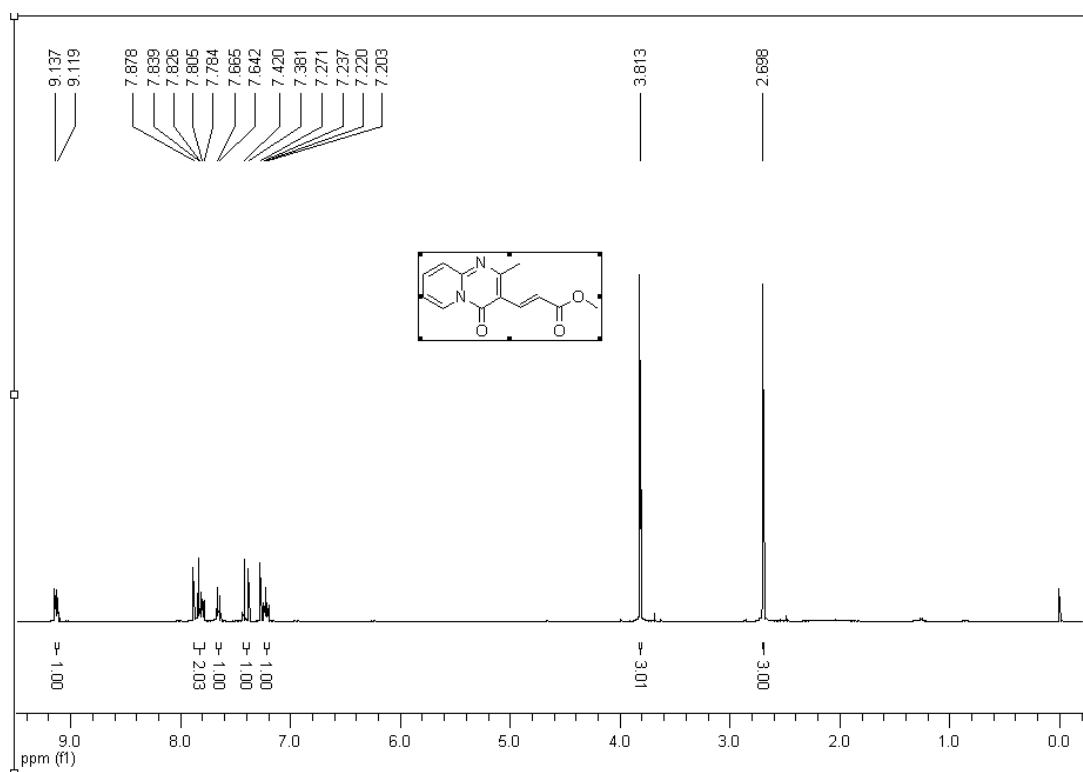
(E)-benzyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3c)



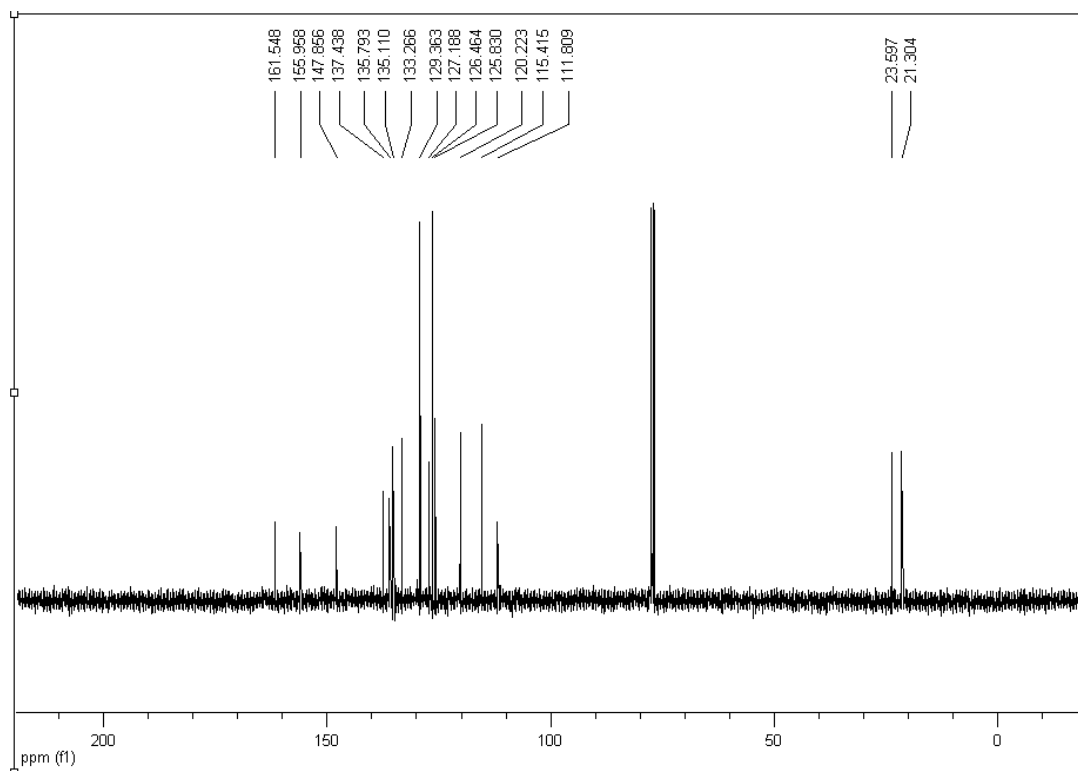
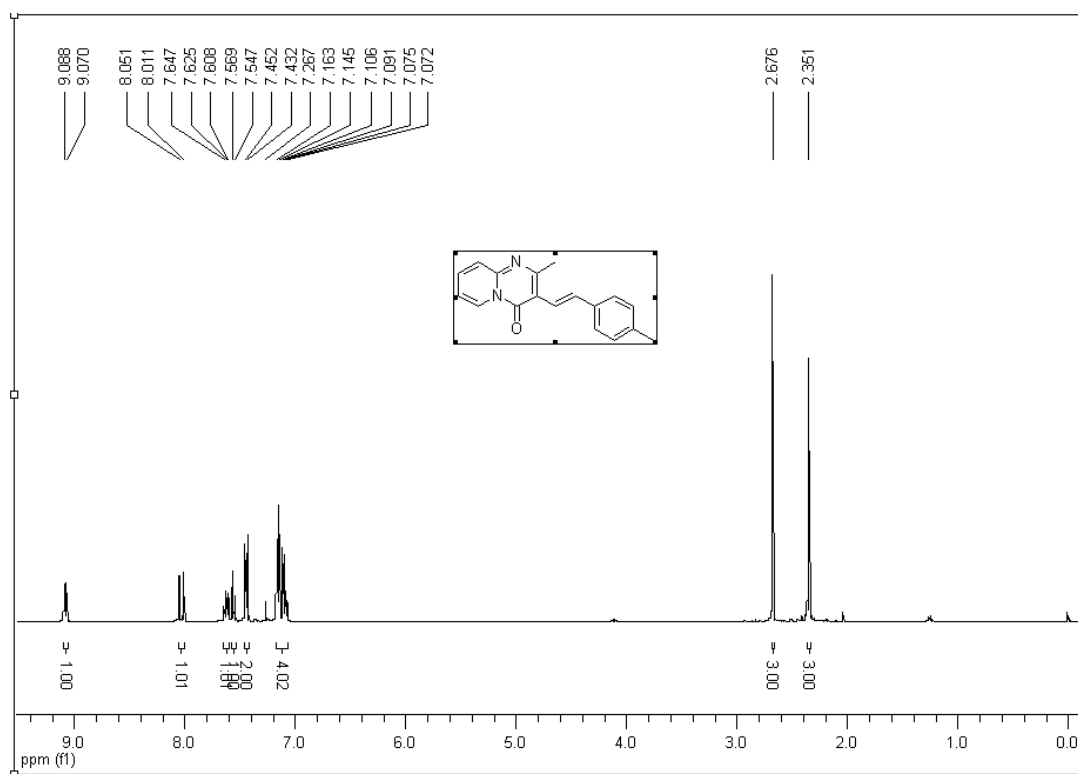
(E)-ethyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3d)



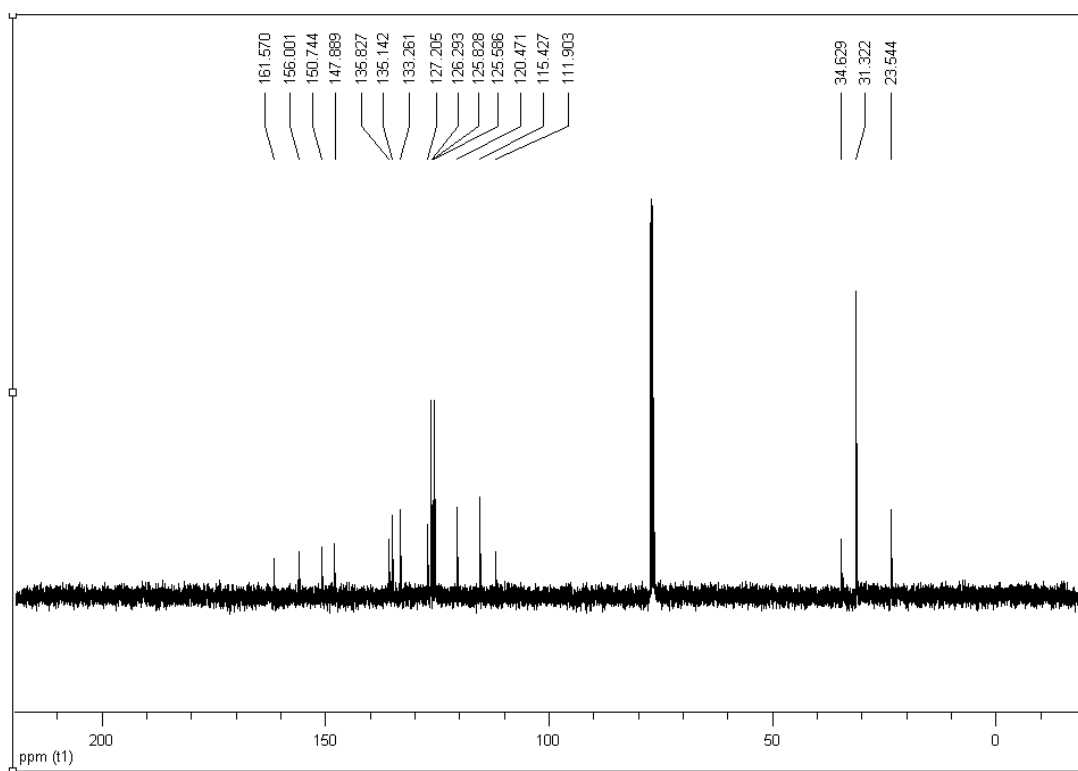
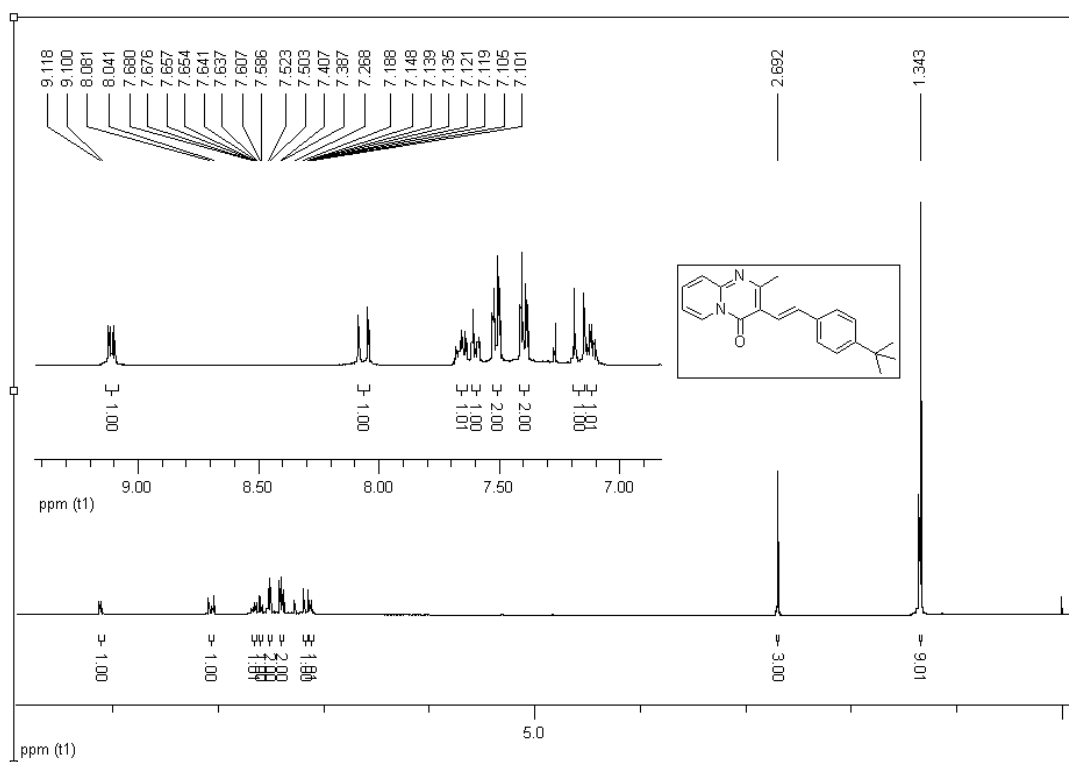
(E)-methyl 3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3e)



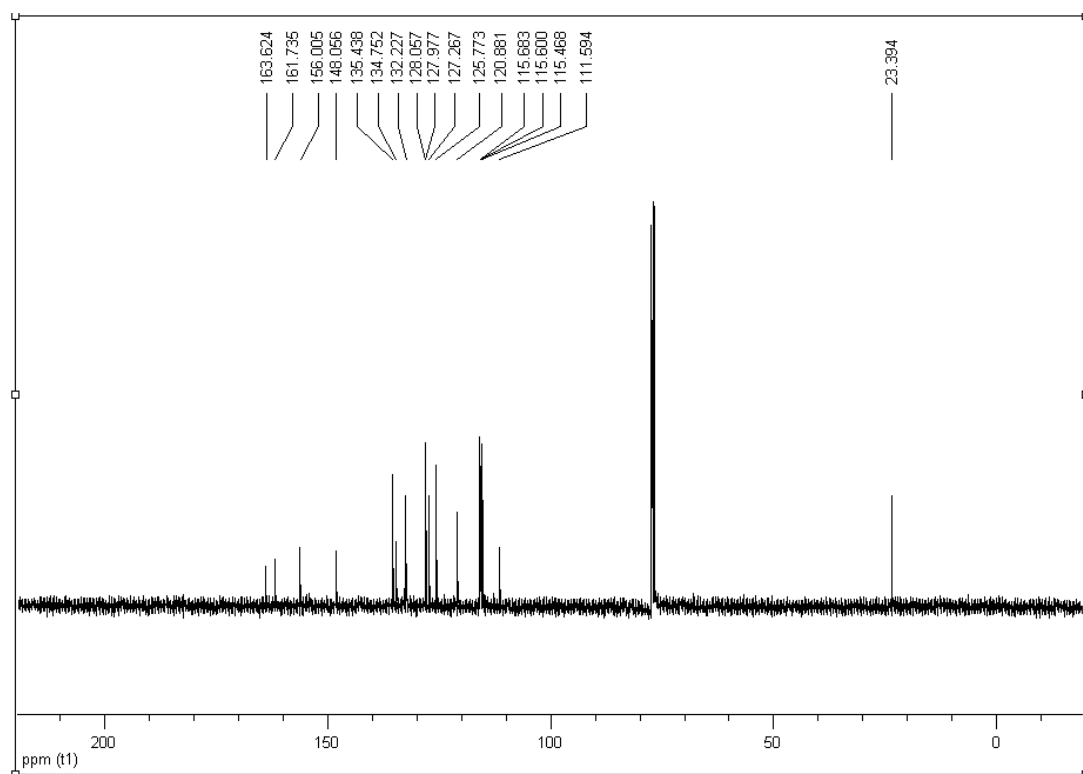
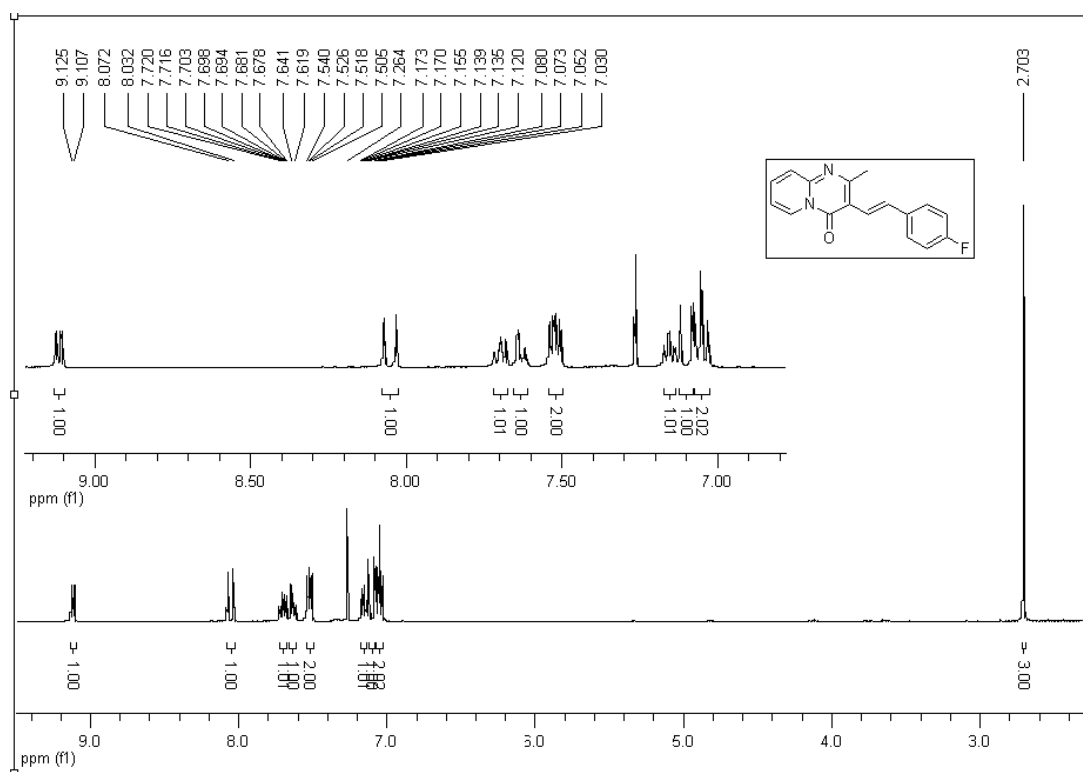
(E)-3-(4-methylstyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3g)



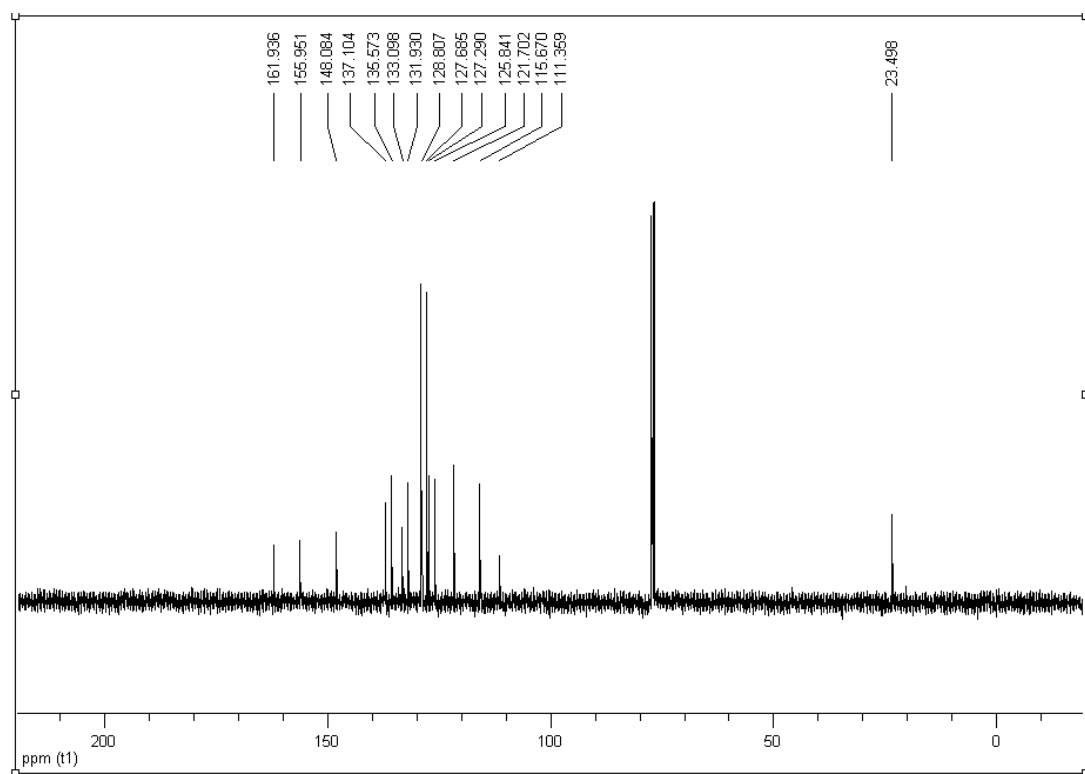
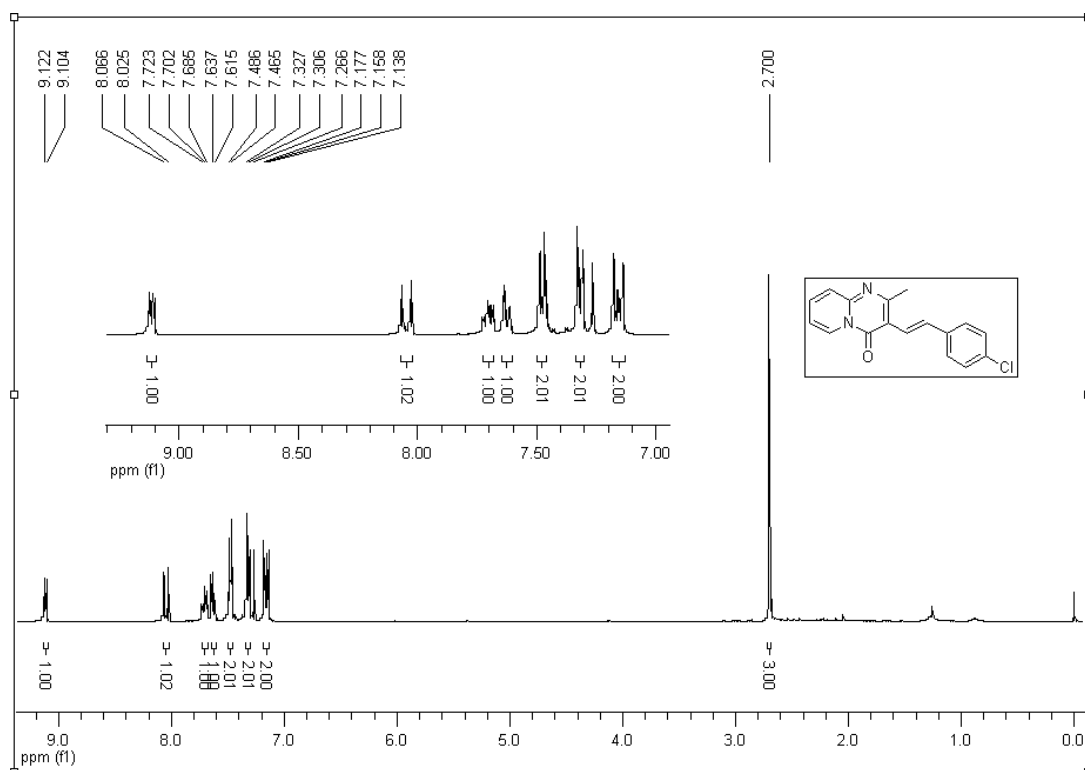
(E)-3-(4-tert-butylstyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3h)



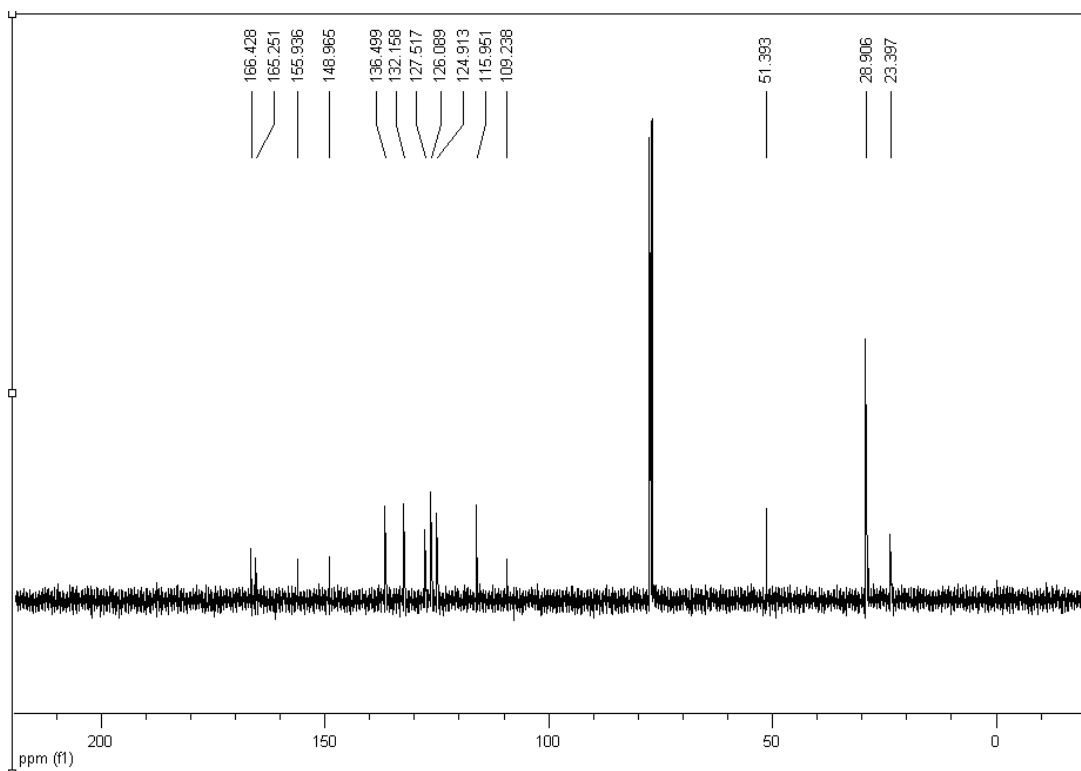
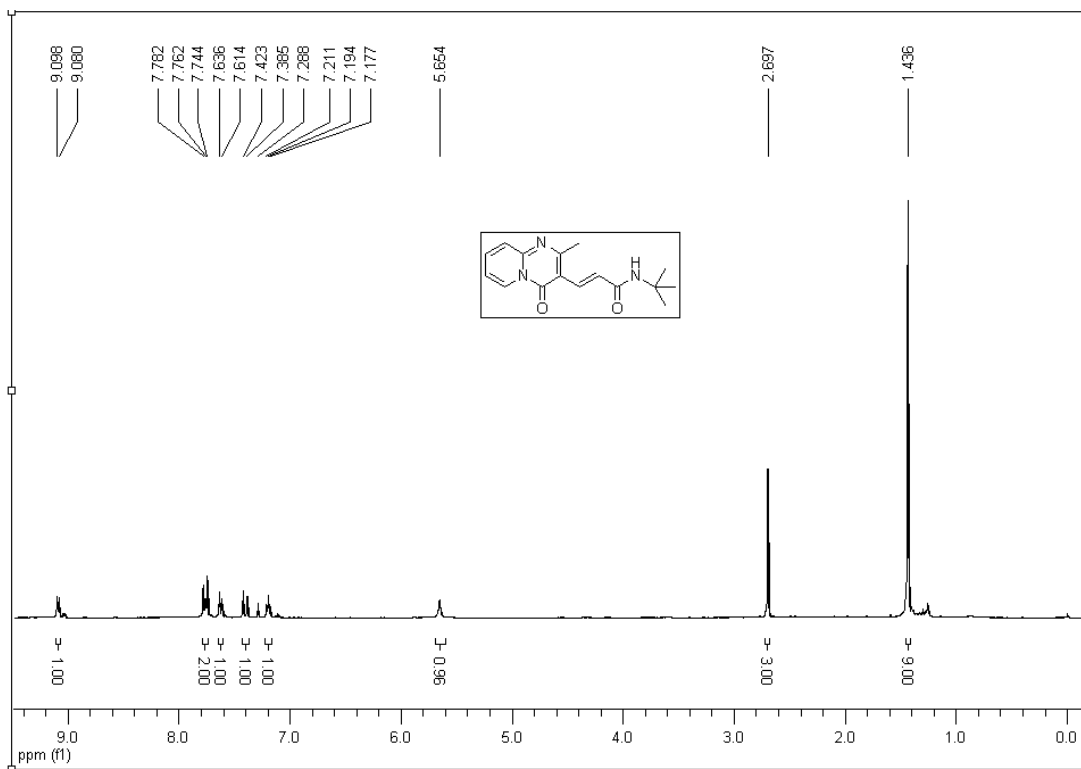
(E)-3-(4-fluorostyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3i)



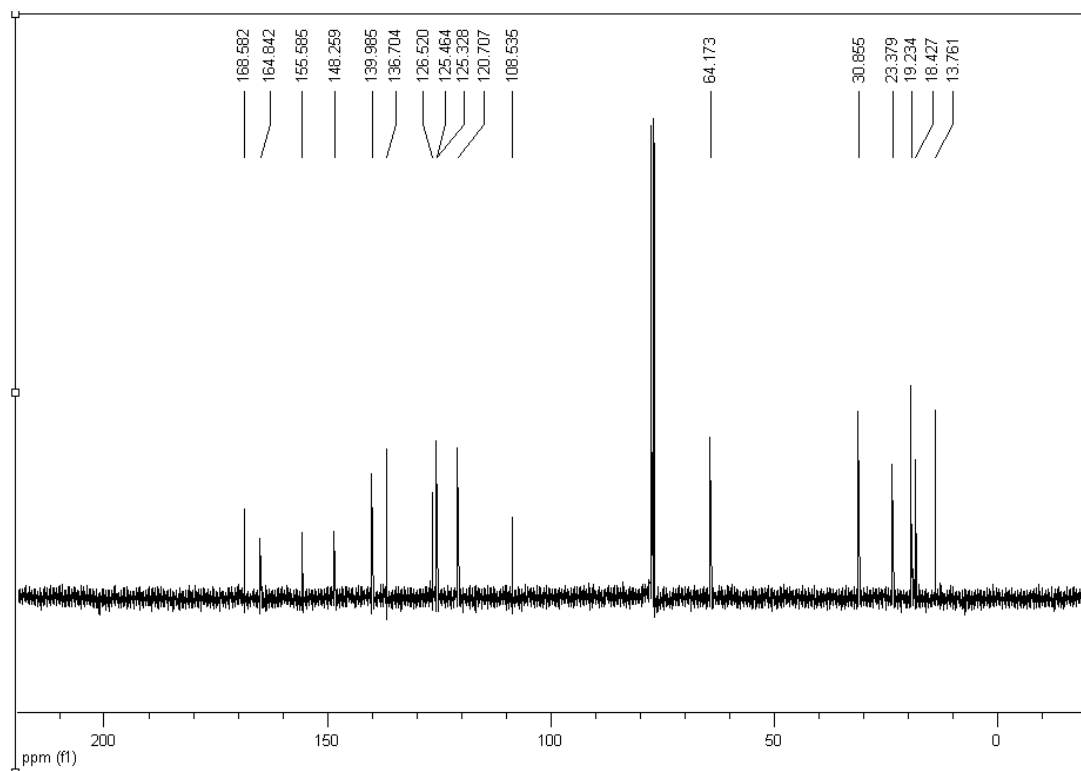
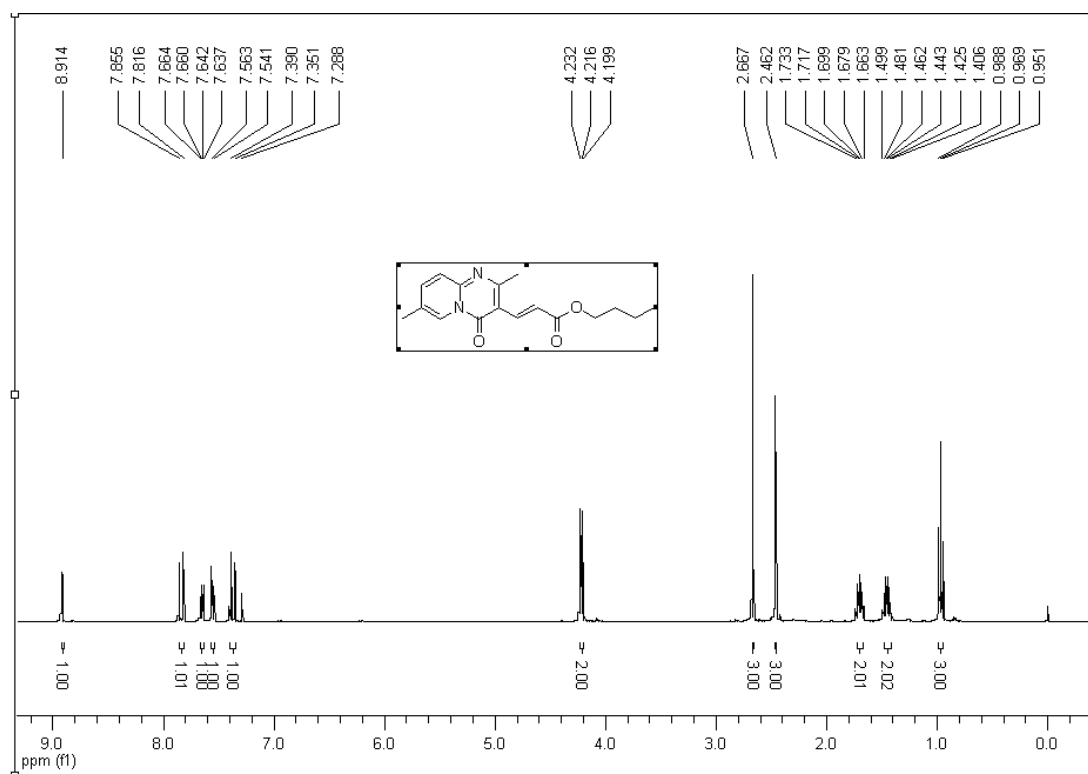
(E)-3-(4-chlorostyryl)-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one(3j)



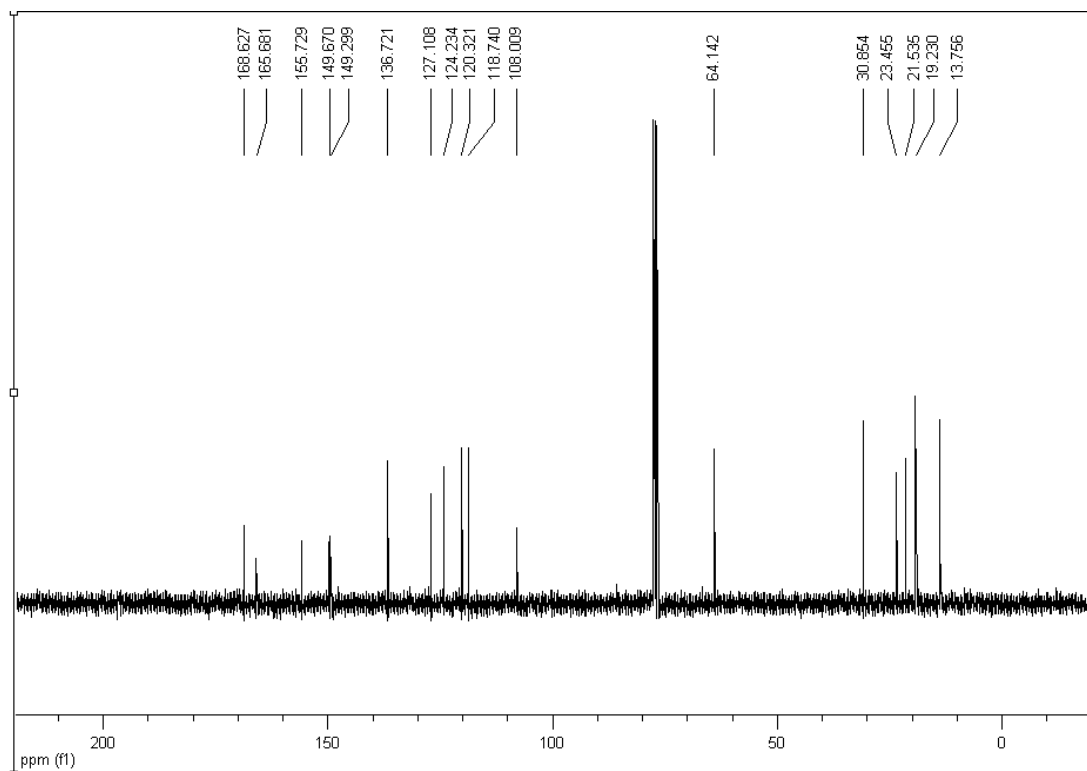
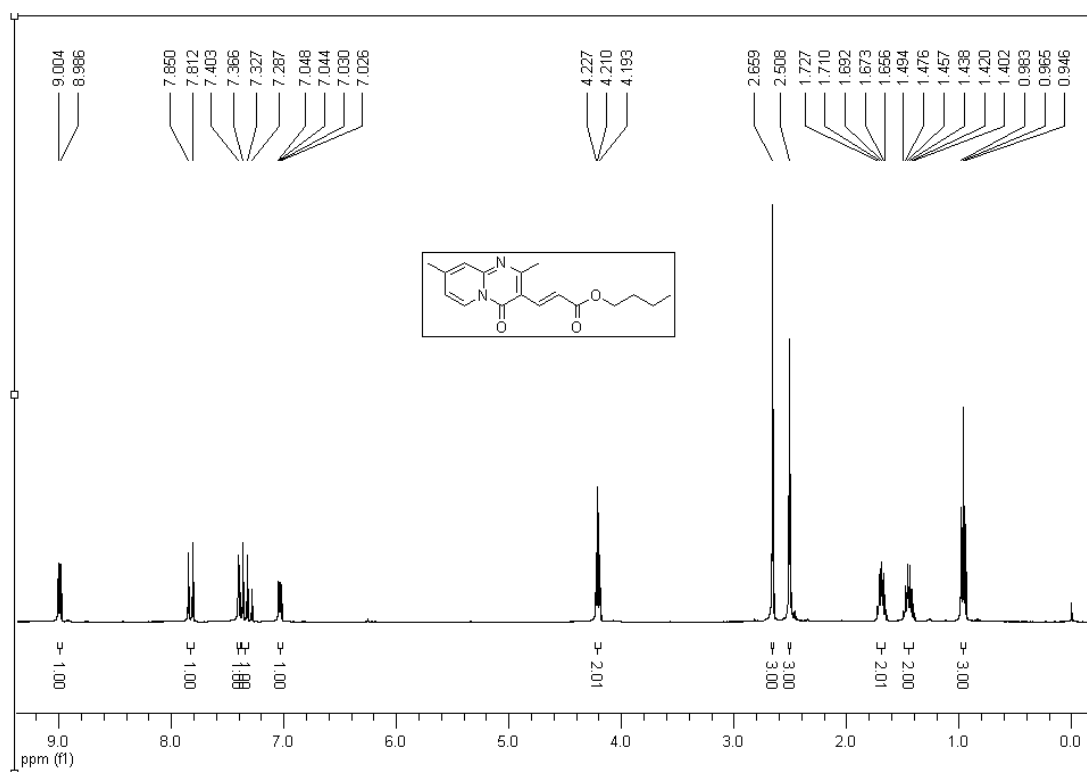
(E)-N-tert-butyl-3-(2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylamide(3k)



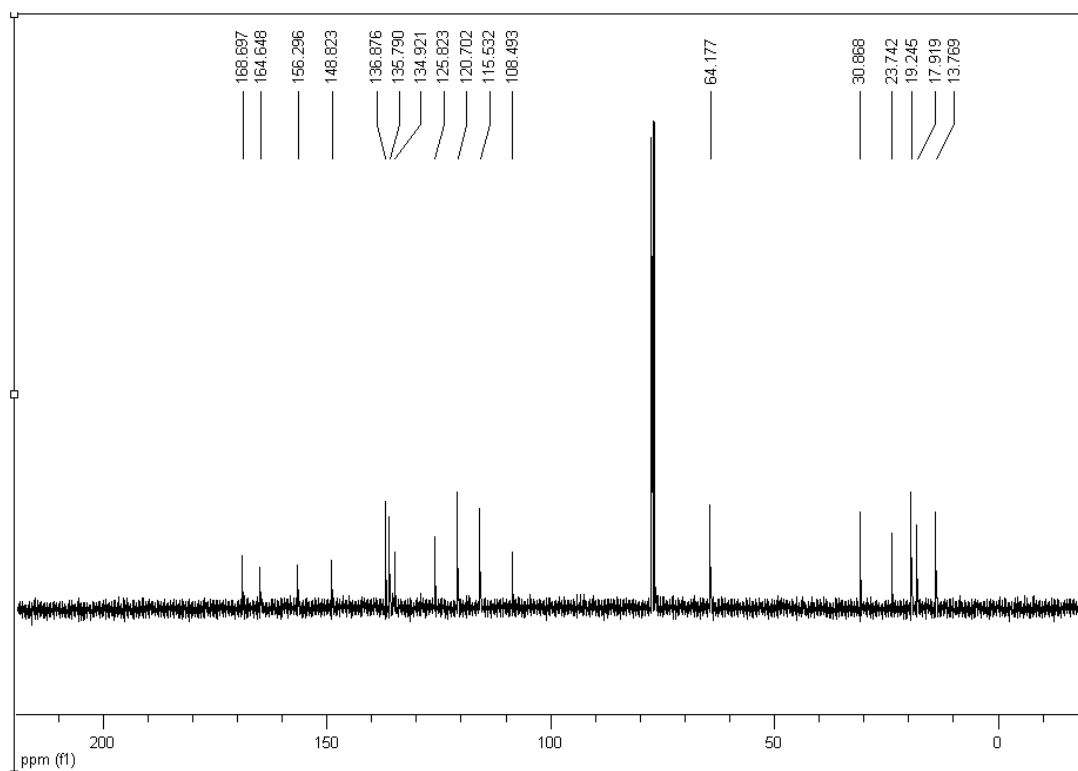
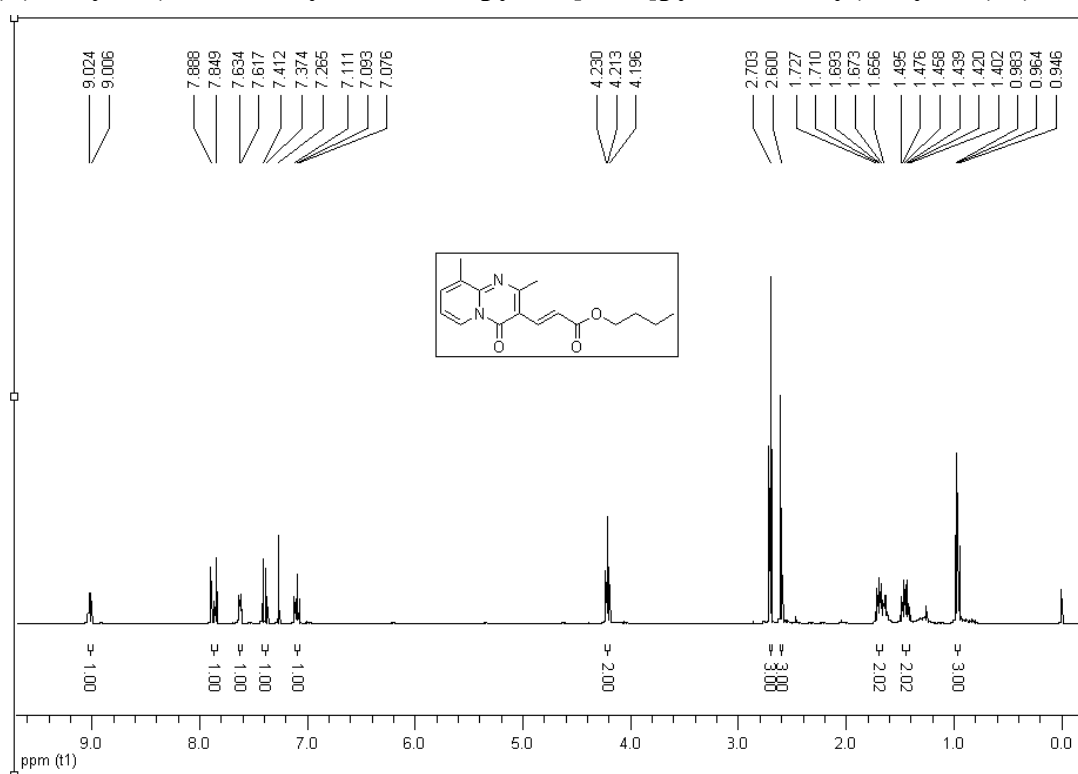
(E)-butyl 3-(2,7-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3I)



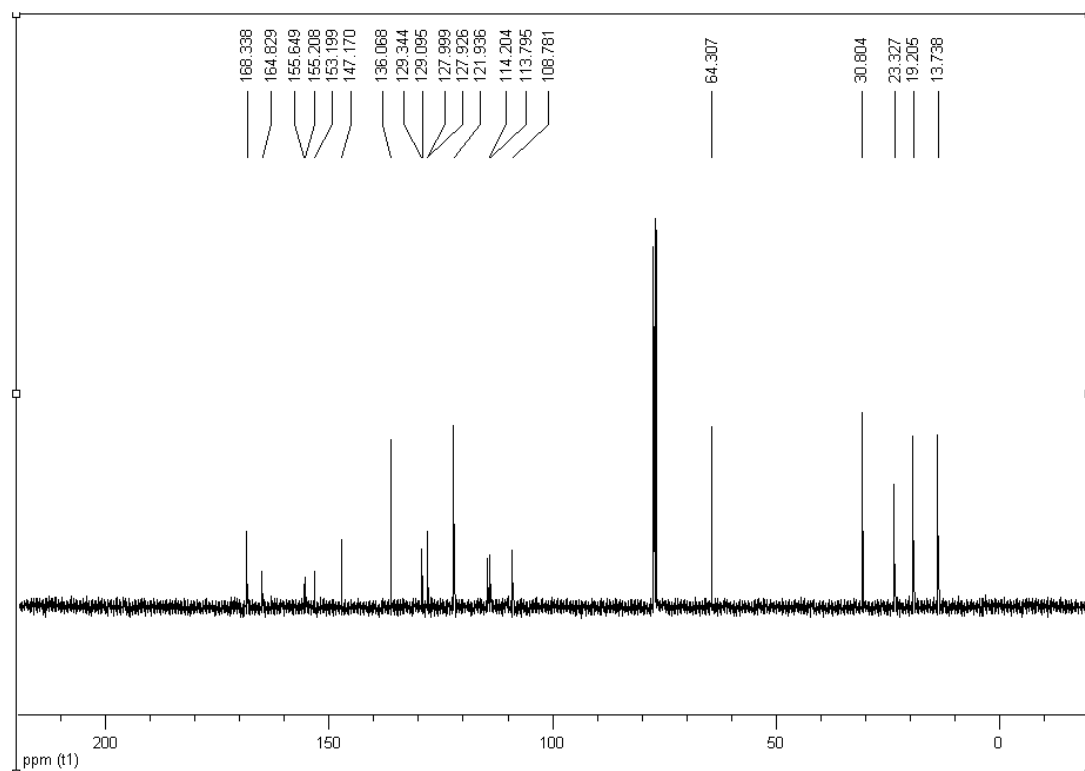
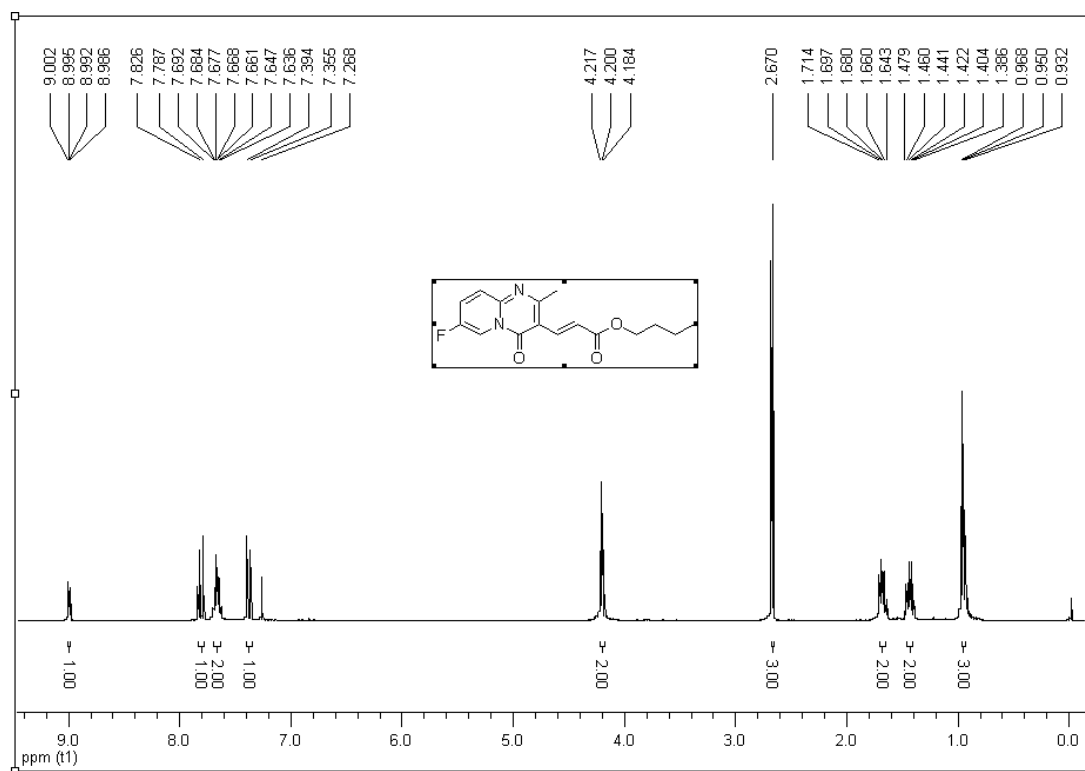
(E)-butyl 3-(2,8-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3m)



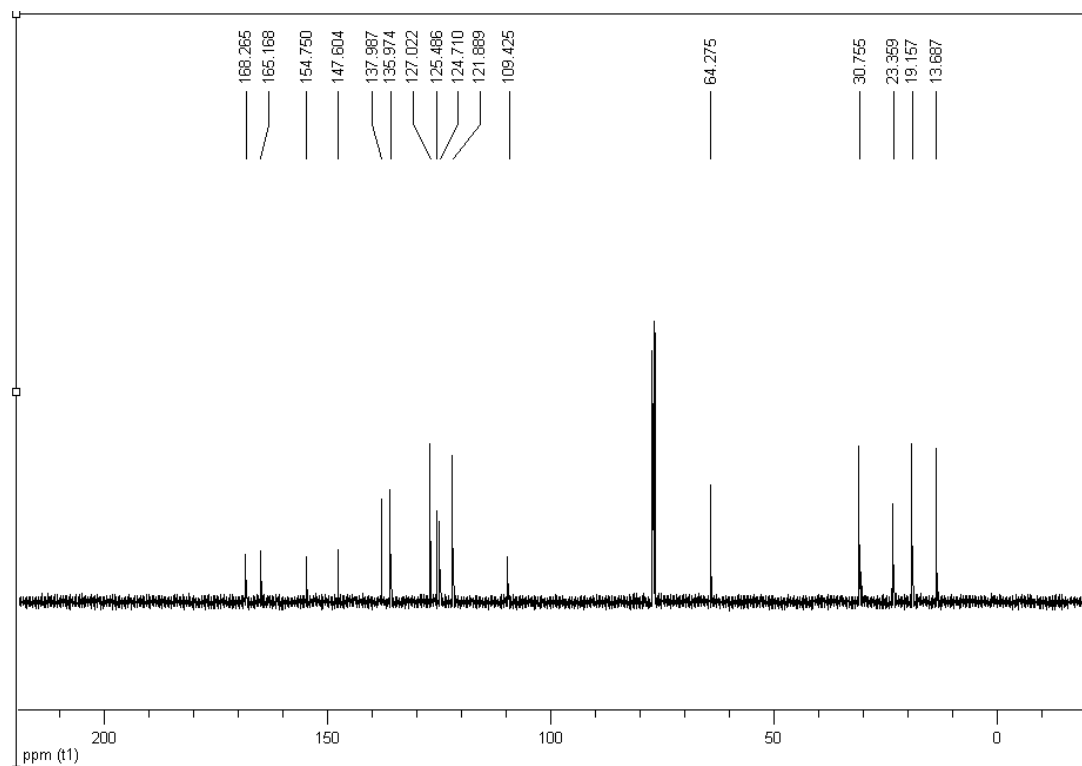
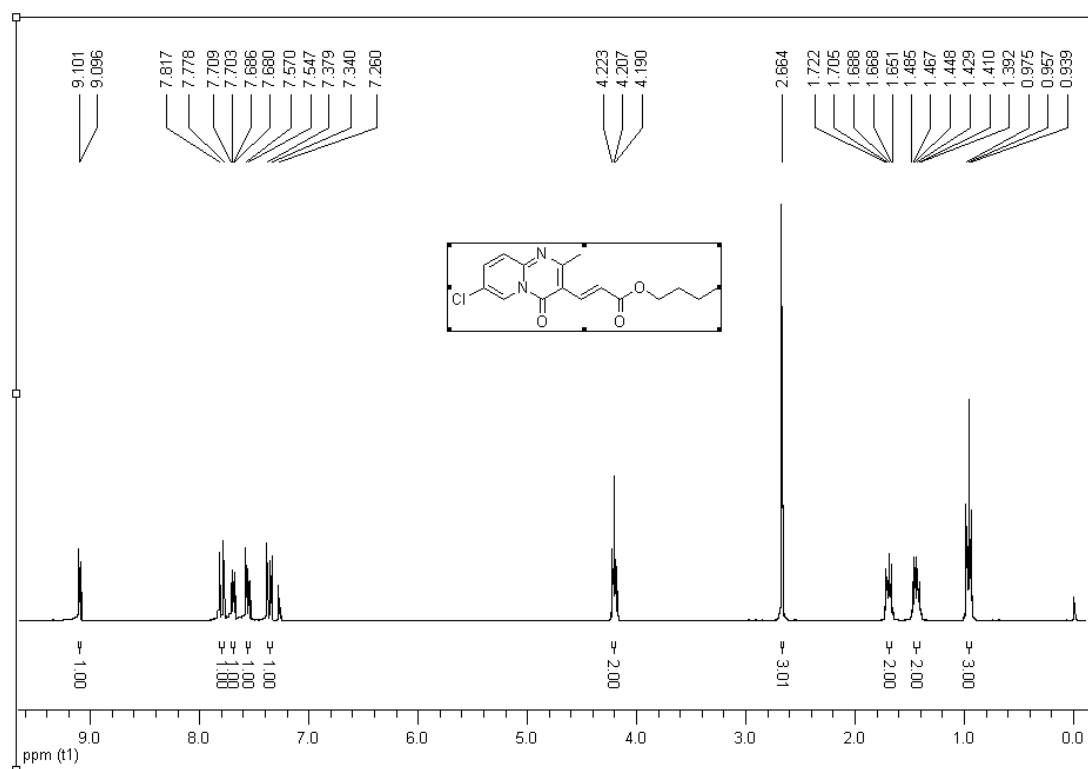
(E)-butyl 3-(2,9-dimethyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3n)



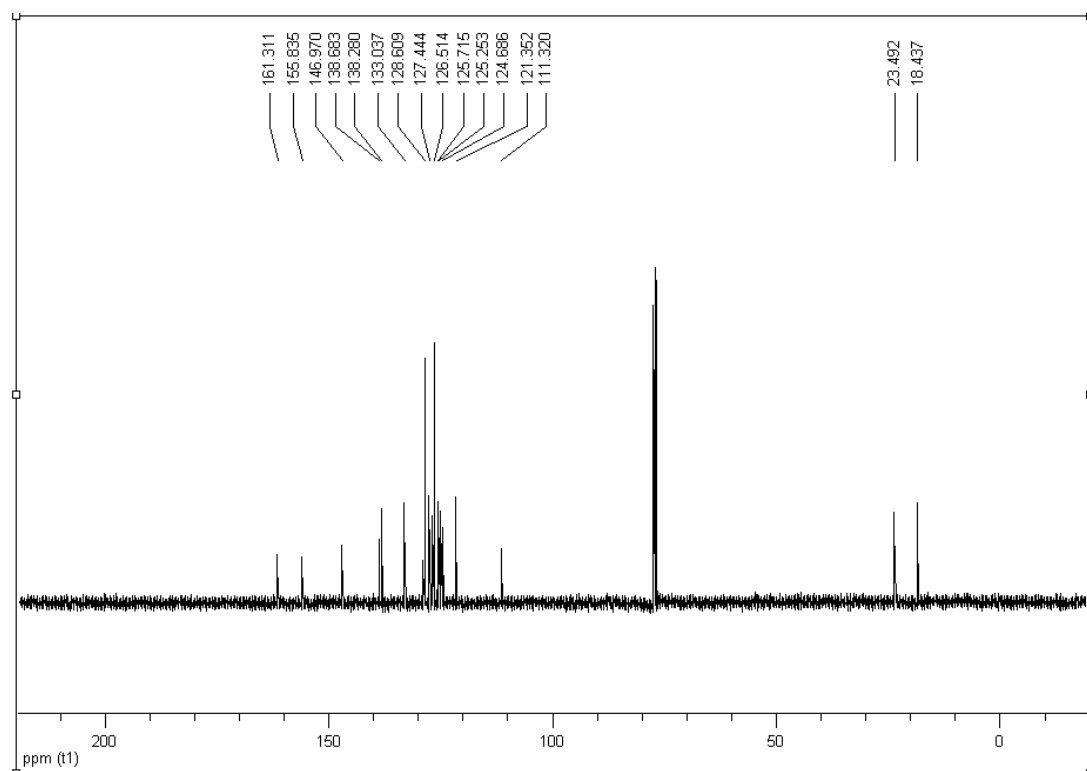
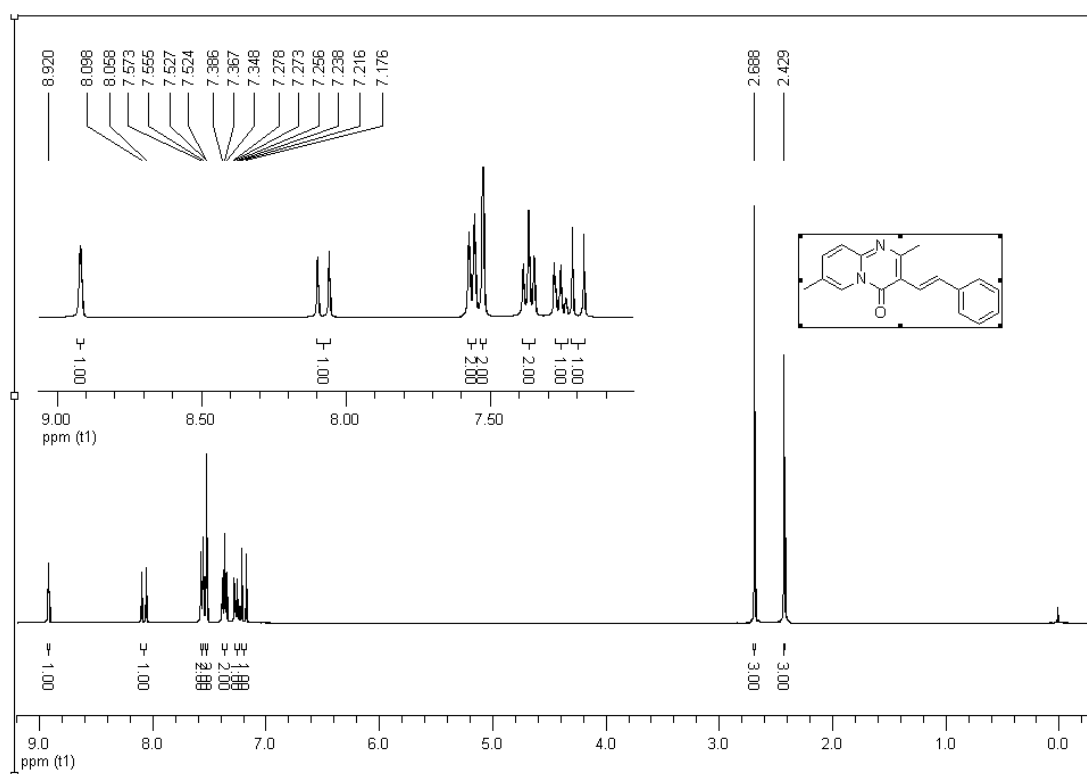
(E)-butyl 3-(7-fluoro-2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3o)



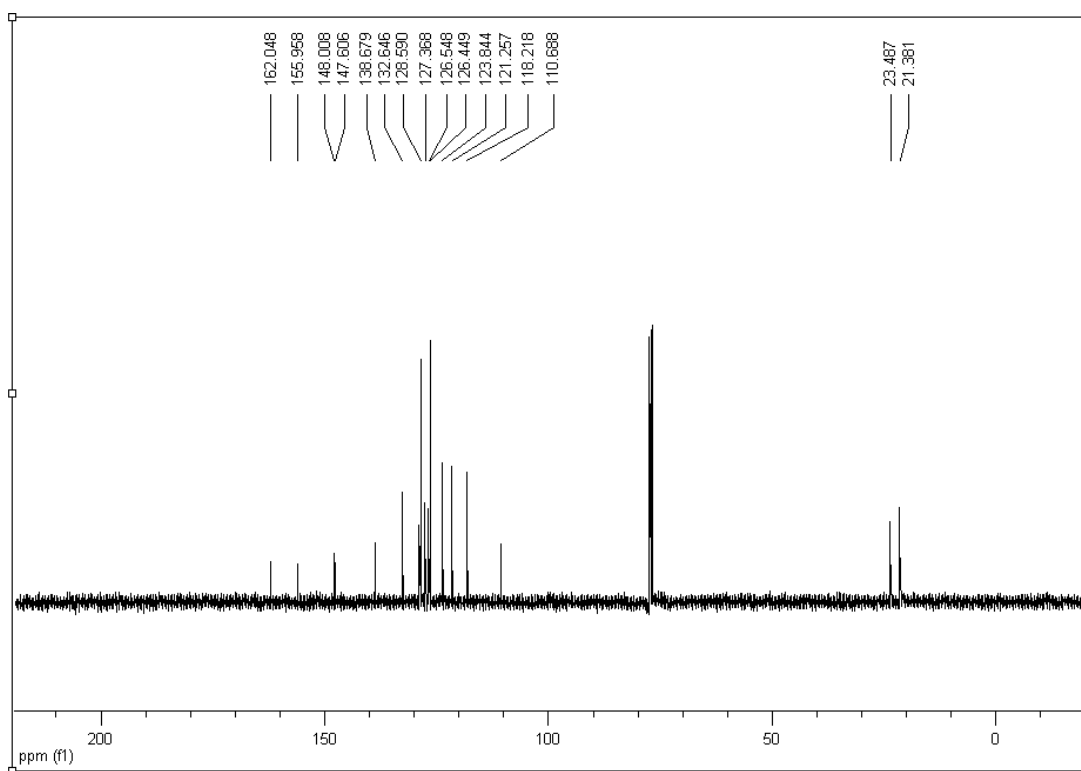
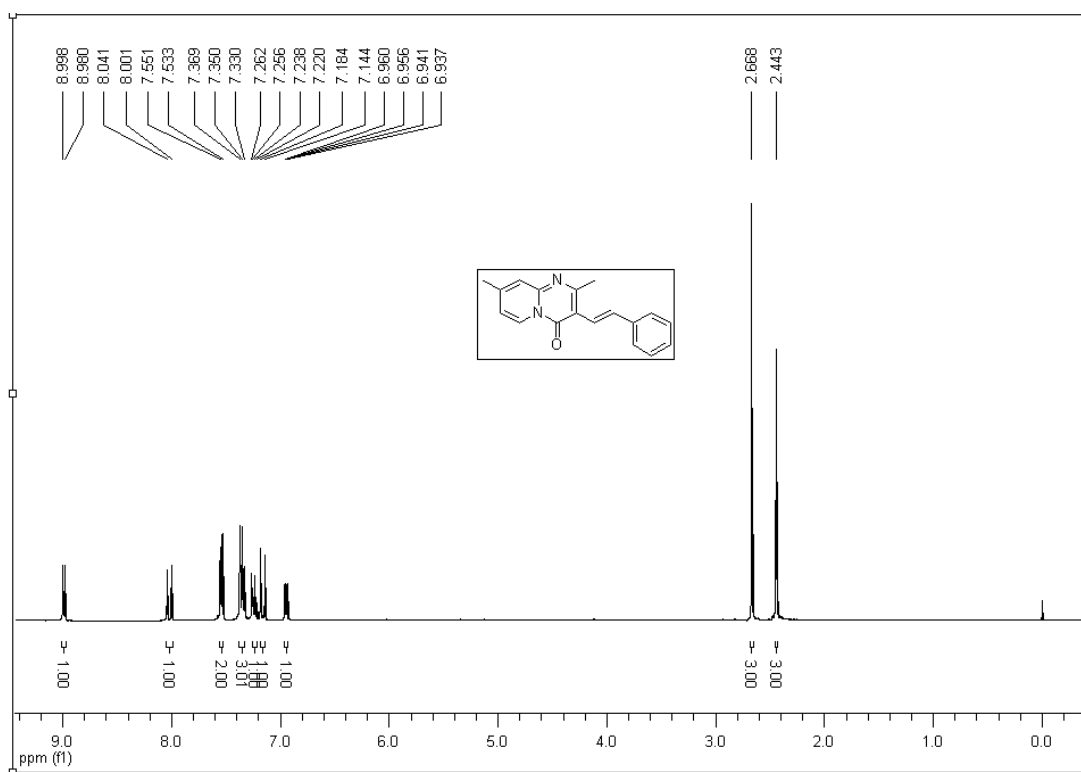
(E)-butyl 3-(7-chloro-2-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-3-yl)acrylate(3p)



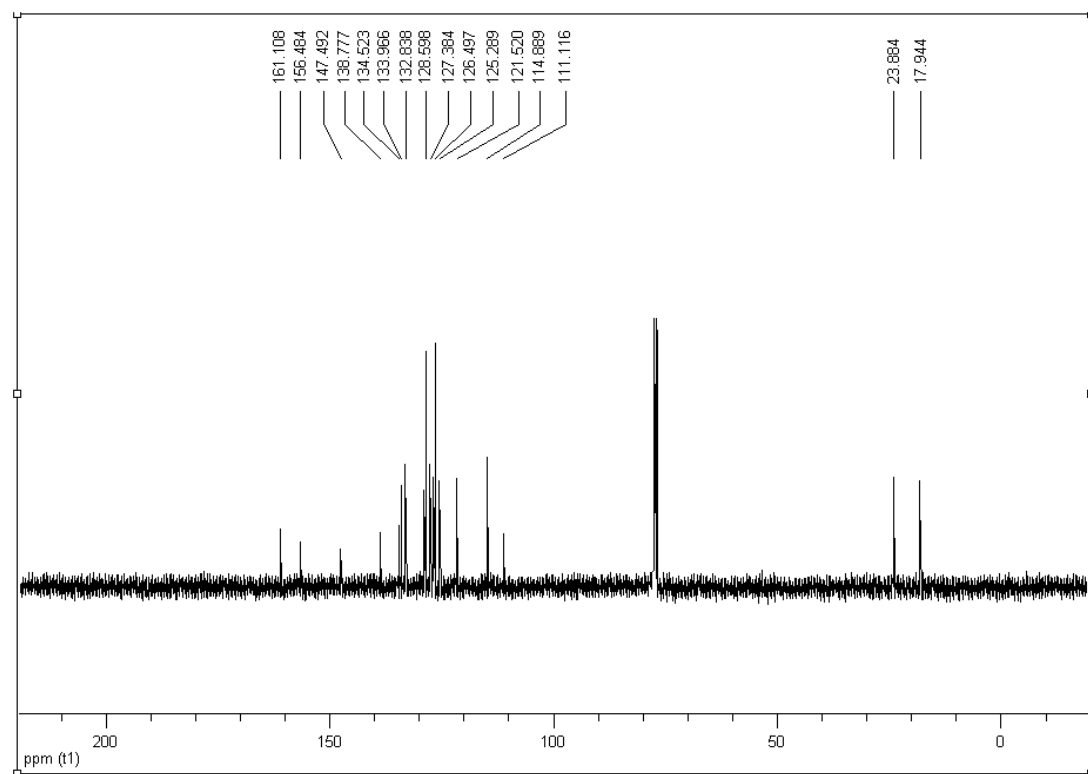
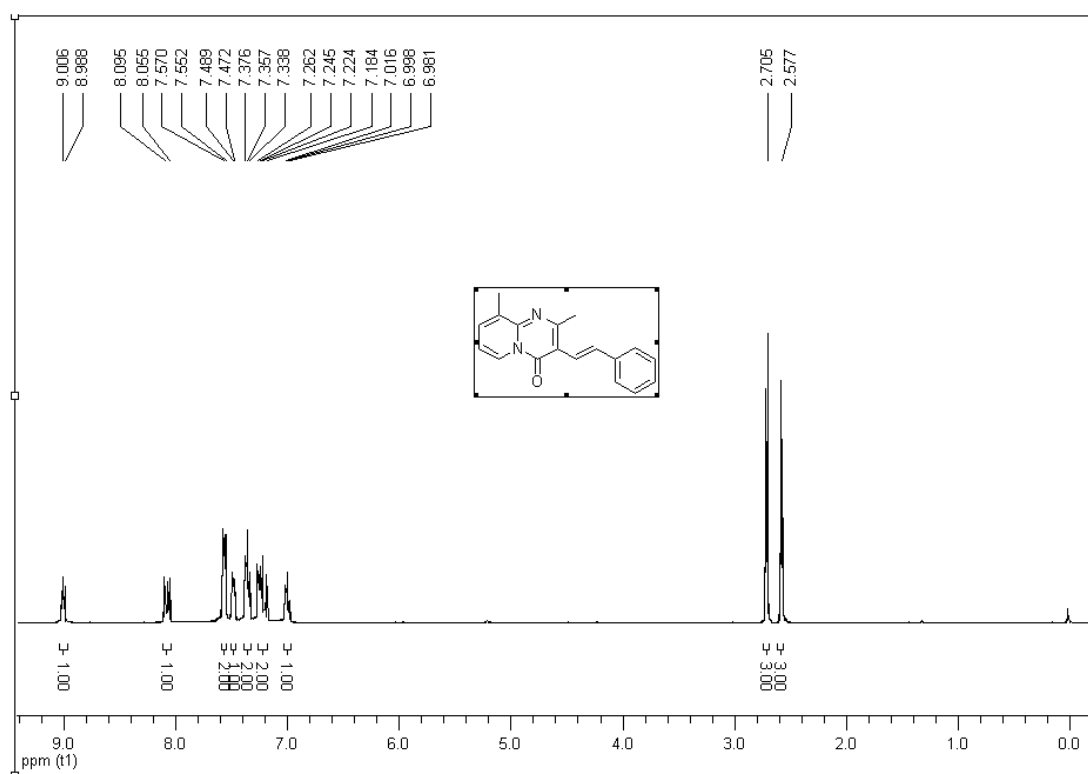
(E)-2,7-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3q)



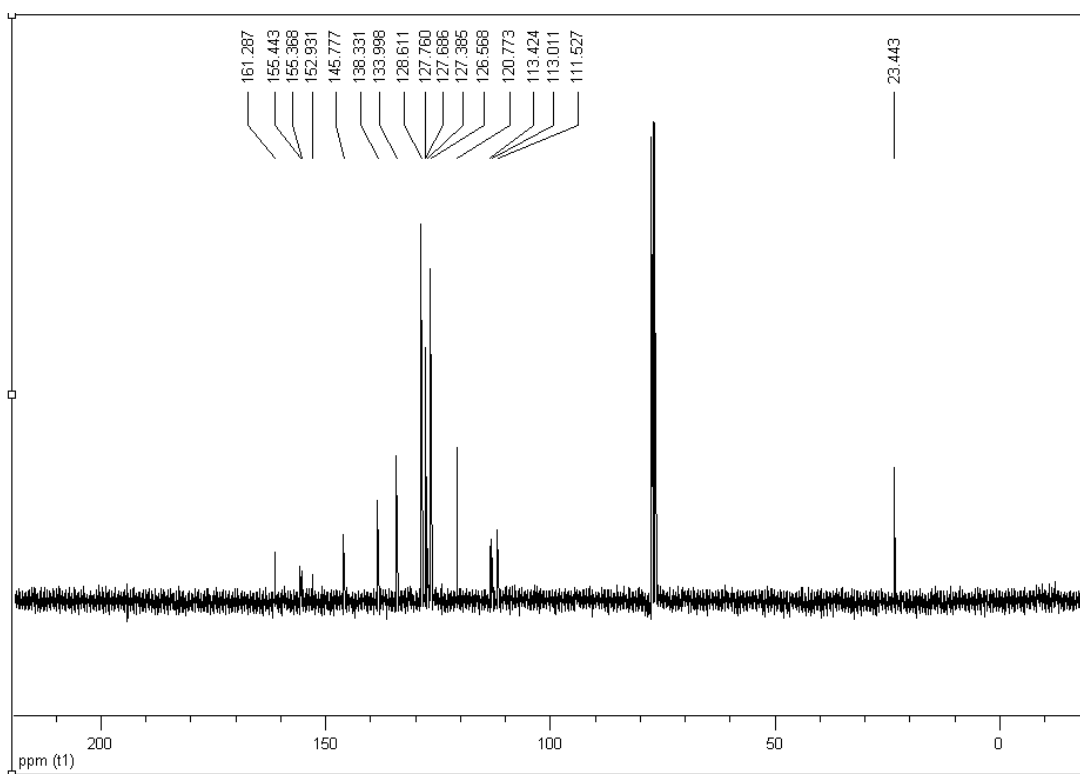
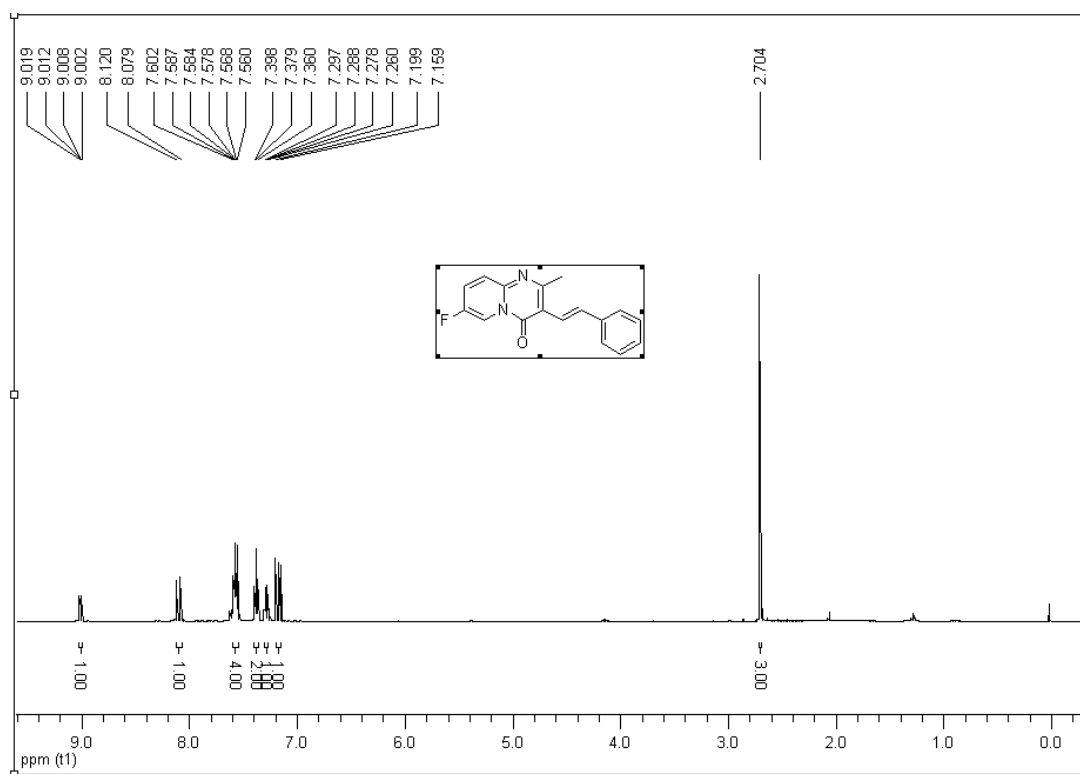
(E)-2,8-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3r)



(E)-2,9-dimethyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3s)



(E)-7-fluoro-2-methyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3t)



(E)-7-chloro-2-methyl-3-styryl-4H-pyrido[1,2-a]pyrimidin-4-one(3u)

